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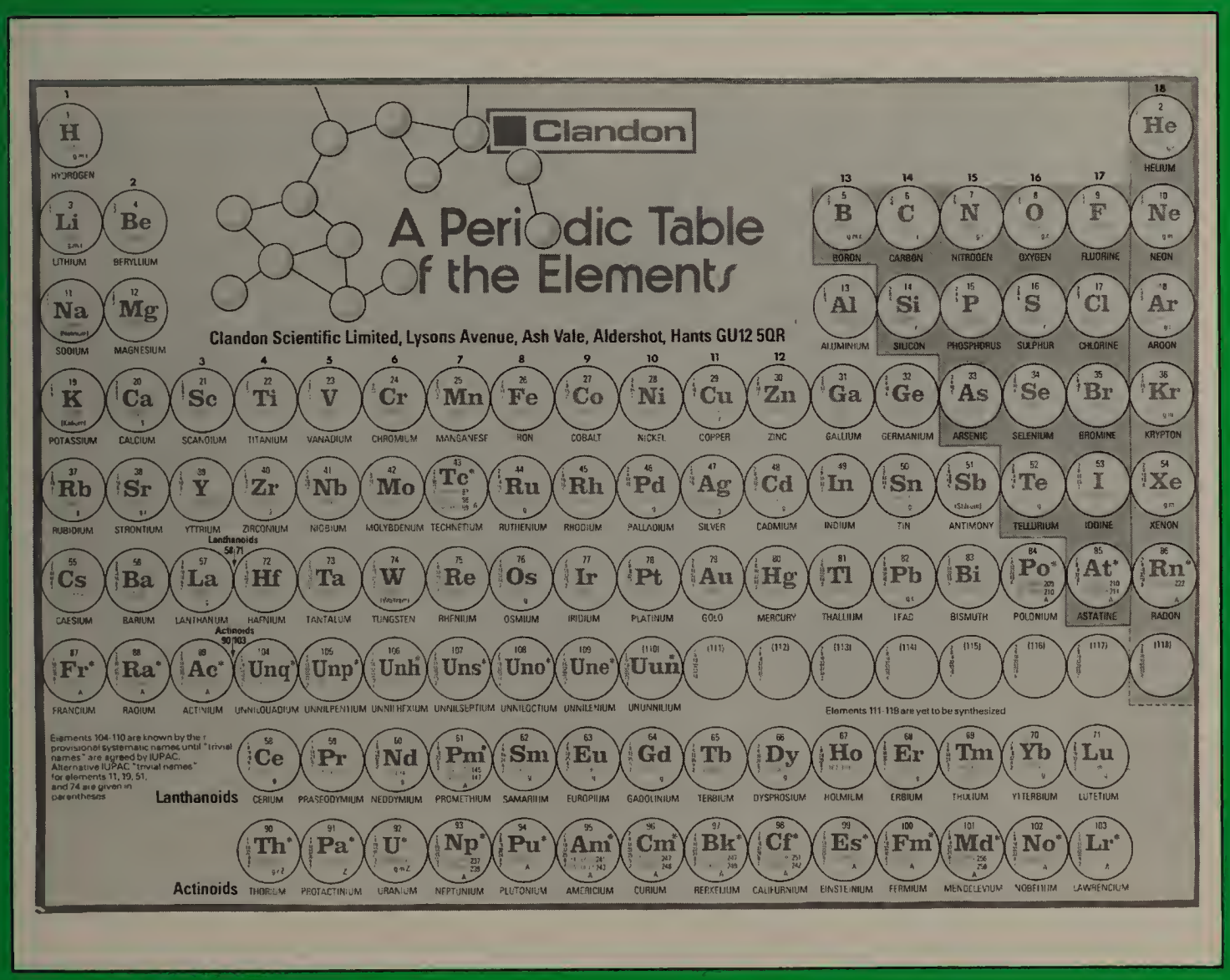
Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)


Clandon
A Periodic Table of the Elements
Clandon Scientific Limited, Lysons Avenue, Ash Vale, Aldershot, Hants GU12 5QR
Lanthanoids
Actinoids
Elements 111-118 are yet to be synthesized
Elements 104-110 are known by their provisional systematic names until "trivial names" are agreed by IUPAC. Alternative IUPAC "trivial names" for elements 11, 19, 51, and 74 are given in parentheses

IUPAC

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Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

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Front cover: Periodic table of the elements. IUPAC has now finalised the names of the transfermium elements from 100 to 109, inclusive.

History of IUPAC 1919–1987

This book by Roger Fennell describes the origins and history of the International Union of Pure and Applied Chemistry up to 1987. Such a history of the Union had been suggested long ago, indeed, a tentative attempt on the history of the first 50 years was made by Stig Veibel, however, the current very detailed work has been almost ten years in preparation.

We are reminded in the *Foreword* written by Professor Kirill Zamaraev, the current President of IUPAC, that IUPAC is a voluntary nongovernmental, nonprofit organization that unites chemists from all over the world. The object of the Union is to contribute to the advancement of both pure and applied chemistry.

It was this desire for international co-operation amongst chemists, and to facilitate the work of the international, but fragmented, chemistry community that was one of the earliest characteristics of the Union. Indeed, even before the creation of IUPAC (1919), the body out of which the Union developed, International Association of Chemical Societies (IACS), had met in Paris in 1911 and produced a set of proposals for the work that the new Association should address. These included:

- Nomenclature of inorganic and organic chemistry;
- Standardization of atomic weights;
- Standardization of physical constants;
- Editing tables of properties of matter;
- Establishing a commission for the review of work;
- Establishing a commission for a universal language;
- Standardization of the formats of publications;
- Measures required to prevent repetition of the same papers.

1911 might seem an early date for chemists to start talking about the possibility of, indeed, need for, international collaboration. However, we are told in this informative book that the first international attempt at organizing, for example, organic chemical nomenclature, the Geneva Nomenclature of 1892, grew out of a series of international meetings, the first of which was organized by Kekulé in 1860.

It is interesting to consider the above list of desirable goals with the advantage of history. Nobody would disagree that the standardization of weights, measures and symbols is essential to the well-being and continued success of the scientific enterprise. This process of standardization and harmonization, in chemistry, has been the task of IUPAC and one it continues to pursue.

The world before the outbreak of World War I was very different from that of the present. Today, the very idea of establishing a commission to decide upon the choice of a universal language would be fraught with political and social problems. The fact that Anglo-American has become not only the *lingua franca* of science, but also of international commerce and trade, has more to do with the events of the middle of our century than a group of eminent and learned men calmly meeting in Paris, discussing the relative merits of different languages for scientific publication.

It is true to say that of all the goals of standardization desired by the IACS, and inherited by IUPAC, only two have not been followed to the present day. Unfortunately, the two points related to the standardization and nonduplication of publications still continue to bedevil the world of research. Different journals have different formats and requirements, and there is still an immense amount of duplication of research, which in these days of ever shrinking research budgets is a cause of concern. It is amusing to speculate that if these early recommendations had been strictly followed, the present world of scientific publishing would be very different, with perhaps fewer journals and consequently smaller and less expensive libraries.

Unfortunately, the outbreak of World War I in 1914 stopped all moves towards closer international scientific collaboration. Indeed, IACS did not recover from the war and in 1919 it was dissolved in favour of IUPAC.

It is clearly seen how IUPAC has, over its 75 years of existence, been a powerful force for the creation of a world-wide chemistry community, a community which knows no borders between nations. IUPAC helps chemists overcome borders and shows how the world community of chemists can act as a team, whatever the

Professor K.I. Zamaraev, Russia, IUPAC President 1994–95.

IACS, Brussels, 1913; (back row) Crossley, Casares, Wauters, Crismer, Auerbach, Hoogewerff, Petersen, Bjerrum, Biilmann, Mourelo, Kurnakow, Ogialoro; (middle row) Fichter, Cohen, Lowry, Walden, Jacobson, Menozzi, Behal, Witt, Hauser, Marie; (front row) Tschugaeff, van Laer, Werner, Guye, Haller, Ramsey, Ostwald, Paterno, Hanriot, Frankland.

political situations in their respective countries. This was particularly the case when war, or the threat of war, loomed large. The Union survived World War II, with activities recommencing, even before the cessation of hostilities, in November 1944 with the restoration of postal services between France and the US. The Secretary General J. Gérard communicating with Union President Marston-Taylor Bogert outlining the work which had been carried on during hostilities. During the Cold War, the Union served as an important channel for intercontinental collaboration.

This book is full of fascinating facts and the stories of dedicated chemists who gave much of their time to help establish and to assist the international chemistry community. For example, we learn that in the first half century of its existence the Union had only three Secretary Generals.

With the Union in such fine form containing many dedicated people, and with such a tradition of individual dedication, the future might seem to be assured and looking bright indeed. However, these are times of unprecedented financial cutbacks in research and development all over the world. Indeed, the numbers of young people seeking to study chemistry is falling. To counter this tragedy, chemists must seek to improve the public perception and support of chemistry. This is certainly difficult, how does one reach the public and government officials and convince them that chemistry is vitally important. Unfortunately, for many members of the public, the word chemistry elicits antipathy and fear, with visions of dumps of toxic waste and cancer-causing agents. Yet, the chemical industry is still enormously important to the world economy and there continues to be ever more numerous demands for new and more versatile materials. We as chemists know how important is our discipline, but we must seek to show others that this is the case.

This then is the achievement of IUPAC after 75 years of existence. The creation of a genuinely world-wide community of chemists, both from academia and industry, with pride in what has been accomplished for this community of chemists, together with hope that the chemistry endeavour will continue successfully, with greater public support and perception of the value of chemistry.

History of IUPAC 1919–1987*, by Roger W. Fennell published by Blackwell Science Ltd, Oxford, 1994. xiv + 354 pages, ISBN 0-86542-878-6 (hardback) GBP24.95/USD39.50 is available from Blackwell Science Ltd. A paperback version (ISBN 0-86542-879-4), is available at a reduced rate, GBP6.26/USD10.00, through the Oxford Secretariat only to members of IUPAC bodies and Affiliate Members.*

Roger Fennell (left) receiving a copy of the *History of IUPAC* from Simon Rallison of Blackwell Science.

Naming the transfermium elements

A study of the origin of the names given to the chemical elements is sometimes the first romantic attachment formed by young potential chemists with their future career. One is fascinated by the manner in which the various names have been derived. For example, from the name of the naturally occurring mineral from which the element was extracted (sodium, potassium or carbon), or from the locality where that mineral was found (strontium or copper), or from the name of the city were the discoverer lived (hafnium), or from the colour of the purified element (chlorine), or its chemical inertness (argon), or even be derived from the difficulty of extraction from the naturally occurring source (tantalum, lanthanum or dysprosium). One is reminded of Davy and Berzelius isolating and naming practically whole columns of elements.

The naming of the most recently discovered, or perhaps one should say fabricated as they are not naturally occurring having nuclear instabilities, chemical elements has, however, required more international compromise than classical erudition. There has, for example, been much discussion and no little disagreement concerning the discovery of the transfermium elements. To clarify this situation, a Transfermium Working Group (TWG) was set up in 1986 by IUPAC and IUPAP (International Union of Pure and Applied Physics) to consider questions of priority in the discovery of elements with nuclear charge number, Z, greater than 100. The conclusions of this working group were published in two phases by IUPAC, in 1991 and 1993.

In the first phase, it was decided that a set of criteria would be established which would have to be satisfied for the discovery of an element to be recognized. The establishment of these criteria would be undertaken in close collaboration with the laboratories concerned and would not concern individual cases, i.e. individual elements, or priorities. The report on this first phase (Part I) of the TWG report was accepted by IUPAP and by IUPAC in 1990 and published in *Pure Appl. Chem.* **63**, 879–886 (1991) and as a note in *Chem. Intl.* 13, 213 (1991).

The report of the second phase of the Group's work, the critical or judgmental phase, was accepted by the IUPAP and IUPAC councils in 1991 forming Parts II and III of the TWG report. Both parts were published in the August 1993 issue of *Pure Appl. Chem.*(Discovery of the transfermium elements: Introduction to the discovery profiles, *Pure Appl. Chem.* **65**, 1757–1763, Discovery of the transfermium elements: Discovery profiles of the transfermium elements, *Pure Appl. Chem.* **65**, 1764–1814). Also published with Parts II and III were the responses from the laboratories most closely concerned (Joint Institute for Nuclear Research, Dubna; Gesellschaft für Schwerionenforschung, Darmstadt; and Lawrence Berkeley Laboratory, California, USA), together with the reply to these responses by TWG.

In this second phase of its work, the TWG applied the criteria established in Part I, on an element-by-element basis, it considered all the available literature and discussed, in chronological and critical detail, those publications considered to be important in the first observations of each new element. This delineation of discovery profiles resulted, in some cases, in a sharing of the credit for discovery. A summary of the conclusions of the TWG on the priority of discovery of the transfermium elements can be found in *Chem. Intl.* **16**, 16–17 (1994).

After publication of its deliberations, TWG ceased to exist, however, it recognized that the responsibility for naming the transfermium elements must rest with the IUPAC Commission on Nomenclature of Inorganic Chemistry (II.2). This Commission met in Balatonfüred, Hungary, on 31 August 1994 to consider the naming of

Einstein and Bohr in Brussels during the 1930 Solvay Congress. Both have now been honoured with chemical element names.

the transfermium elements, 101–109 inclusive. The Commission consisted of twenty chemists, all with equal voting rights, from twelve countries. The debate was wide-ranging, thoughtful and objective, as it should be considering the significance of the process to chemistry in general.

Beforehand, the three major laboratories involved in the discoveries had been asked for their proposals concerning the naming of the elements and the reasons for their choice. The Commission considered these proposals and deliberated upon the precedents for naming elements. It was unanimously agreed to continue the practice of naming elements after appropriate scientists, places and properties. However, it resolved, by a substantial majority, that an element should not be named after a living person. The majority felt that it was necessary to have the perspective of history in relation to these discoveries before any final decision could be taken. The Commission showed itself to be sensitive to the suggestions from the three laboratories as to the choice of individual names, that is, to the choice of scientists or laboratory to be honoured. All the names finally chosen came from the suggested lists, however, not necessarily in the order suggested. The final list is as follows:

Element	Name	Symbol
101	Mendelevium	Md
102	Nobelium	No
103	Lawrencium	Lr
104	Dubnium	Db
105	Joliotium	Jl
106	Rutherfordium	Rf
107	Bohrium	Bh
108	Hahnium	Hn
109	Meitnerium	Mt

The recommendations of the Commission as a whole were ratified unanimously by the Titular Members.

For elements 101–103, the Commission accepted the *status quo*. Mendelevium is named after Dimitri Mendeleyev who devised the periodic table. The element was discovered in 1955 by bombarding unweighably small quantities of einsteinium with helium nuclei. It was just possible from these experiments to identify the presence, two or three atoms per bombardment, of a new element. Nobelium is named in honour of Alfred Nobel. A 1957 claim of discovery was disputed, but nobelium was positively identified in 1958 by the Berkeley group. Observations were not made on the element itself, but on atoms of fermium

The Solvay Physics Council, Brussels 1911. Seated from left to right: Nernst, Brillouin, Solvay, Lorentz, Warburg, Perrin, Wien, Mme Curie, Poincaré. Standing from left to right: Goldschmidt, Planck, Rubens, Sommerfeld, Lindemann, de Broglie, Knudsen, Hasenohrl, Hostelet, Herzen, Jeans, Rutherford, Kamerlingh Onnes, Einstein, Langevin.

Irène et Frédéric Joliot-Curie.

250, a daughter atom produced by nobelium's decay. Lawrencium, named after Ernest Lawrence, was discovered in Berkeley by bombardment of californium with boron in a chamber fitted with a copper conveyer; the new atoms (one at a time) were carried to a radiation detector for identification.

Element 104 was named to recognize the distinguished contributions to chemistry and nuclear physics made by the international research centre at Dubna near Moscow; the element was synthesized by bombarding californium with carbon nuclei. The name joliotium was chosen to honour the French scientist F. Joliot-Curie who shared the 1935 Nobel Prize for Chemistry with his wife, Irène Curie, for the discovery of artificial radioactivity. Irène was the daughter of Marie and Pierre Curie, who were also both Nobel Laureates. Element 105 was synthesized by bombardment of californium with nitrogen nuclei.

Elements 106 and 107 were named after Ernest Rutherford (New Zealand and UK) and Niels Bohr (Denmark), respectively, to recognize their immense contributions to the development of Twentieth Century physics and chemistry.

Naming the adjoining elements 108 and 109 after Otto Hahn (Germany) and Lise Meitner (Austria) honours their decisive role in the discovery of nuclear fission. Lise Meitner thus becoming only the second female scientist to be so recognized by having an element named in their honour; curium ($Z = 96$) being named after Marie Curie and her husband Pierre. These heavier elements have been synthesized by a cold fusion technique in a linear accelerator. The process is slow, requiring a week of bombardment of a suitable target nucleus to produce a single atom which exists only for a fraction of a second.

In choosing names of eminent, but deceased, scientists for the names of elements 105–109, IUPAC has avoided the thorny suggestion of the name 'seaborgium' for element 106 after Nobel Laureate Glenn T. Seaborg (Lawrence Berkeley Laboratory, USA). Following the tradition that the discoverers of an element have the right to suggest a name for that element, members of the Berkeley team, less Seaborg, unanimously suggested the name seaborgium for their newly discovered element. However, as with many of the issues concerning these heavy elements, the name seaborgium has proven controversial. There has, over the last 30 years, been considerable rivalry between the group at Berkeley in the USA and Dubna in Russia, a rivalry in which the Cold War may well have played a part. The two laboratories have made competing claims for the discovery of a number of the transfermium elements (see *Chem. Intl.* **16**, 16–17 (1994).

The above recommendations were unanimously accepted by the IUPAC Bureau at its meeting in Antwerp, Belgium, in September 1994 for submission to the International Committee on Nomenclature and Symbols as definitive for publication in *Pure Appl. Chem.* They are subject to ratification by the IUPAC Council when it meets at Guildford, UK, in August 1995.

Nobel Prizes for 1994

George A. Olah of the University of Southern California has won this years Nobel Prize in Chemistry. Olah, 67, a naturalized US citizen emigrated from Hungary in 1956 and worked at Dow Chemical and Case Western Reserve University before moving to USC in 1977.

The Swedish Academy awarded the prize for his studies of carbocations, positively charged species that are a common intermediate of many organic reactions.

In the 1920s and 1930s as chemists began to figure out the mechanisms of organic reactions, it became clear that carbocations were involved in many reactions as intermediates. Indeed, the nature of these intermediates was a long standing dispute. For example, the structure of the 2-norbornyl cation fascinated many physical organic chemists. The late Saul Weinstein of Harvard argued that the cation contained pentacoordinated carbon; Herbert C. Brown of Purdue maintained that the cation was a rapidly equilibrating trivalent carbon species.

Olah used the Lewis super-acid SbF_5 to extract halide ions from alkyl halides in solvents that were such poor nucleophiles that they did not readily attack the positively charged hydocarbon species. Olah found that such super-acids (10^{18} times stronger than concentrated H_2SO_4) are so strong that they can force normal tetravalent carbon atoms to accept an additional proton, producing pentacoordinated carbocations. In this way, Olah found a means of stabilizing these transient species long enough to perform spectroscopic measurements, such as NMR and ESCA, and identify the carrier of the spectra. The term carbonium ion had long been used for any hydrocarbon cation. Olah suggested reserving it for pentacoordinated cations and using the term carbenium ions for trivalent cations. Carbocation would refer to either cation, as is now generally accepted. In the case of the 2-norbornyl cation in a solution of SbF_5-SO_2ClF-SO_2F_2, at –158 °C, the NMR spectra showed the cation to be bridged carbonium ion as suggested by Weinstein.

The ability to protonate or extract a proton from a hydrocarbon may well lead to isomerization, for example, converting straight chain hydrocarbons into branched hydrocarbons, which boosts the octane rating of hydrocarbon fuels. Such isomerizations are commonly believed to occur in solid super-acids such as zeolites.

This year's physics prize was shared between Bertram Brockhouse (McMaster University, Canada) and Clifford Shull (MIT, USA) for the development of instrumental techniques, diffraction scattering and inelastic scattering, in neutron scattering.

Neutron diffraction works in much the same way as x-ray diffraction; the fact that the de Broglie wavelength of thermal (defined by the velocity of the neutron) neutrons is of the same order of magnitude as the spacings between atoms in crystals, without the damaging effects of the high-energy X-ray photons, means that neutrons are particularly well suited to probing problems in materials science. Also, the intensity of scattered X-rays is determined by the average electron content of the scattering atom. Consequently, there is little discrimination between the scattered intensity from organic crystals. Carbon, nitrogen and oxygen scattering with much the same intensity and hydrogen atoms are essentially transparent – little electron density. Neutrons, however, scatter in proportion to properties of the nuclei of the target atoms, not the electronic cloud around the nuclei. So in neutron scattering, hydrogen atoms have by far and away the largest scattering cross section – in a bound state they are essentially just a nucleus. Neutron scattering is then a technique ideally suited for probing the presence and dynamics of hydrogen atoms in solids.

The neutron has another advantage over the photon in that it is magnetic. The neutron has an intrinsic spin and will therefore behave just like a small magnet. Consequently, when a beam of polarized neutrons, that is, all the individual magnetic moments pointing in the same direction, is incident upon a magnetic solid, either a bulk magnet or a paramagnetic salt, there is a particularly strong interaction. Indeed, one of the great triumphs of neutron scattering has been the development of magnetic scattering studies of inorganic and organic magnetic materials.

Likewise, a neutron incident upon a molecule can exchange energy with that molecule. Indeed, energy can be taken up by the neutron from the molecule or given to the molecule from the neutron and subsequent analysis of the energy, that is, velocity, of the neutron, after scattering, reveals both Stokes and anti-Stokes scattering patterns – as in Raman spectroscopy. The difference with photons in Raman spectroscopy, however, is that the neutron is not subject to any selection rule. The nature of the interaction between a molecule and a neutron is very different from that between a molecule and a photon. The result being that in inelastic neutron spectroscopy there are no selection rules to transition probabilities. For example, any vibrational transition which is possible can be observed. This situation has many advantages for the study of new materials.

Neutron scattering is now widely used by chemists, however, it is not a cheap technique. To produce an intense source of neutron requires either a large nuclear reactor, or a spallation source where an energetic beam of, for example, protons hits a heavy metal target. Most neutron scattering centres are therefore international, for example, the Institut Max von Laue-Paul Langevin, Grenoble, France.

The work of the Nobel Laureates in physiology/medicine, Alfred Gillman (University of Texas, USA) and Martin Rodbell (NIEHS, USA) focused on G-proteins. These are so called because they bind guanosine 5´-diphosphate (GDP) or guanosine 5´-triphosphate (GTP). They are cell surface proteins that receive chemical signals from the exterior of a cell and pass the message along intracellularly so that the cell may respond to external stimuli. G-proteins also help convert light signals to visual stimuli in the retina and also play a key role in smell and taste.

Gillman and Rodbell were instrumental in establishing the biochemistry of the systems of regulation and signalization involving these proteins.

Dysfunction of G-protein is now known to play a role in several diseases. For example, cholera bacteria produce a toxin that locks G-protein into the activated GTP bound form, causing salt and water lose, which leads to dehydration and death. Some symptoms of diabetes and alcoholism are believed to involve altered G-protein signalling, and some types of cancer are caused by mutated G-protein.

Medicinal Chemistry

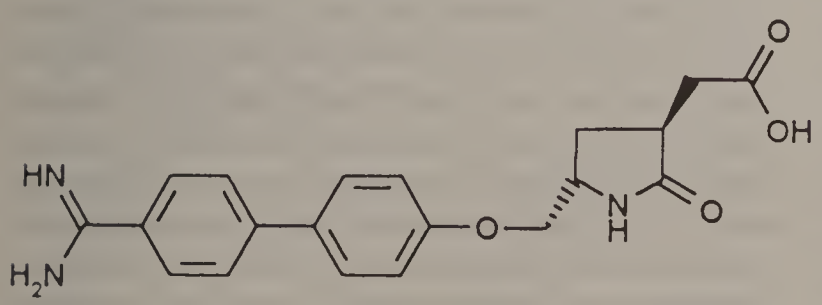
Rational design of pharmaceuticals and agrochemicals has, for the past decade, been the synthetic approach of choice. The idea being that rather than relying on serendipity, chemists would actually design molecules based on their knowledge of structure and activity relationships. Now it appears that that approach may be overtaken by a process called combinatorial chemistry. Delegates at the XIIIth International Symposium on Medicinal Chemistry, held in Paris on 19–23 September 1994, were updated with the latest trends in chemistry.

Pharmaceutical and agrochemical chemistry has for the past two decades been driven by biology – the discovery and description of the biological mechanisms which underlie diseases. Understanding these mechanisms provided pharmaceutical and agrochemical companies with a whole new world of targets. The problem, however, is that it can still take chemists years to come up with a compound to switch these targets on or off and thus stop the disease. The major stumbling block of the rational approach is the lack of a starting point. Combinatorial chemistry may get round the problem.

Combinatorial chemistry is a technology whose time has come. It is going to revolutionize the drug development programmes of the pharmaceutical industry, according to Jack J. Baldwin, vice president of chemistry Pharmacopeia, a US company focusing on the technology. The reason why he believes this is so is because Pharmacopeia and other combinatorial chemistry companies exist to meet the critical need of pharmaceutical and other companies that need access to compounds that are potentially active biologically. Drug companies need a wide variety of compounds, plenty of them and the ability to screen large volumes. Until recently, pharmaceutical companies would acquire lead compounds either from chemical sample collections, natural products or through *de novo* design. Yet none of these approaches really fits the bill. Combinatorial chemistry does, however.

Combinatorial chemistry is a synthetic strategy capable of producing large chemical libraries composed of diverse structural entities built around a common or related molecular scaffold, explained Baldwin. Instead of creating single well characterized products, combinatorial chemistry creates as many products as possible. The process involves many different chemical transformations taking place in parallel, and a lot of the early work involved creating libraries of peptide chains.

Reacting all 20 naturally occurring amino acids with each other, for example, creates a mixture of 400 dipeptides. Repeating that procedure five more times would yield 64 million different hexapeptides. Clearly, making millions if not billions of new chemicals is conceivable, a further step would yield more than 1 billion different heptapeptides. But mixtures of such compounds are useless if the components are neither easily identified or screened for activity. Furthermore,



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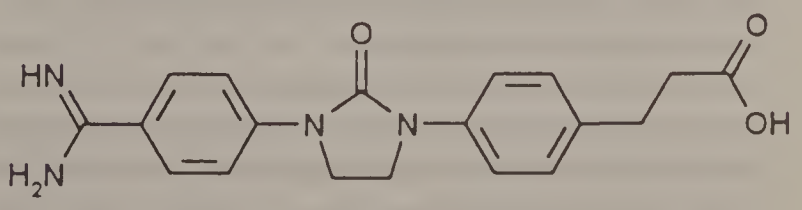

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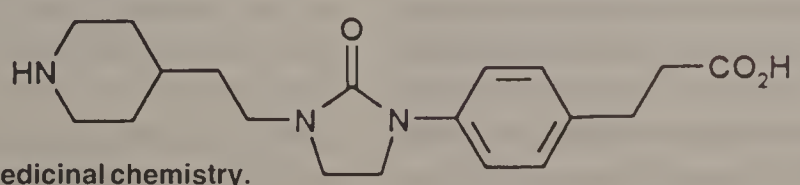
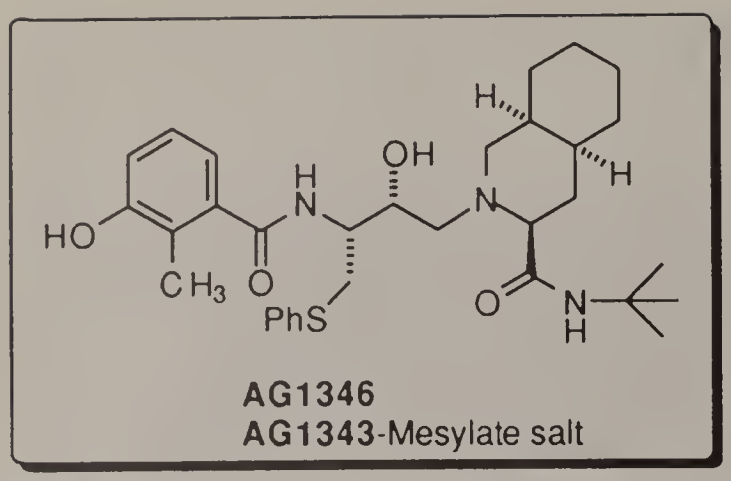


Molecules of current interest in medicinal chemistry.



Molecules AG1346 inhibits HIV-1 protease and displays excellent antiviral activity.

Baldwin noted, use of biological polymers such as peptides or oligonucleotides is restricted owing to the likelihood that any therapeutics that were based on them would not be administered orally and their relatively short half lives.

Pharmacopeia has licensed on an exclusive basis a technology that avoids all the pitfalls associated with combinatorial chemistry, and provides a few added bonuses as well. Pharmacopeia's approach, invented by company co-founder W. Clark Still at Columbia University, in collaboration with Michael Wigler at Cold Spring Harbor Laboratory, is to make small synthetic chemicals and tag each compound with a unique chemical marker. Baldwin describes the tag as a molecular bar code, which can be read using electron capture detection after gas chromatographic separation. The synthesis takes place on an inert bead the size of a talcum powder particle. After each step in a multi-step synthesis for making a combinatorially derived compound, synthetic chemists add to the bead a unique set of inert chemical tags that encode both the step number and the reagents used. After all the steps have been completed, the molecular tags, if necessary, can be decoded within 15 minutes. Unlike other known encoding systems, no co-synthesis is required as the encoding molecules are not connected to one another. This means that the 30 halogenated markers so far produced will allow the synthesis of more than 1 billion different compounds.

The Pharmacopeia approach has been dubbed binary encoding. According to Baldwin, it overcomes nearly all the problems associated with other combinatorial methods. During each step of the split synthesis, a set of chemically stable organic encoding molecules is attached to the beads to encode the step number and chemical reagent(s) used. The array of coding molecules attached to a bead forms a binary encoded record – a molecular bar code of the synthetic operations – tracking reagents, catalysts, reaction conditions – that the bead has experienced and hence encodes the structure of the ligand. The encoding molecules are simple halogenated organics that can be selectively and readily released and are identifiable at sub-picomolar levels by electron capture detection after gas chromatographic separation. Reading the code only requires determining the presence or absence of a given encoding molecule. Baldwin told delegates that the decoding is more rapid that methods using polymerase chain reaction and peptide sequencing and so the number of structures capable of being identified per day per analytical device is 10–100 times that of sequentiable tagging technologies.

Pharmacopeia then can offer the compound libraries it synthesizes to clients looking for lead compounds. These chemicals are then screened, and Pharmacopeia technology permits either screening to be performed with compound library members still attached to their beads, or detached, as well as permitting the testing in the automated 96-well microtitre plate screening format. Any promising lead can then be identified by reading the zip code. Compounds may be synthesized in a totally random way or via a more targeted approach where a basic building block is used initially. This approach will attract the interest of companies developing biologically active molecules for a number of reasons. First, the vast number of new and diverse leads it can generate. Secondly, the speed with which those syntheses, screenings and lead compound identification can be achieved. And third, the sheer cost savings involved.

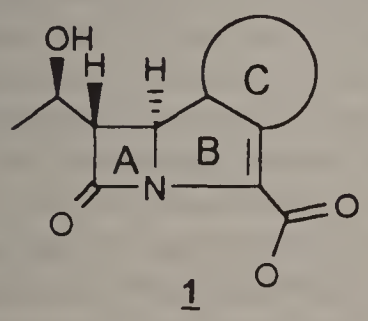
Major pharmaceutical companies have their own libraries of compounds they have either synthesized or collected as natural samples. These will on average contain about 200 000 compounds but they will tend to be in clusters rather than diverse in nature. About half of these compounds will be screened for activity against a particular receptor and promising leads then analysed. The cost for a pharmaceutical company to produce one compound has been calculated to be in the $5000–7000 range. With our knowledge of chemistry, computers and analytical chemistry we can produce new leads faster and less expensively. Already, Pharmacopeia has synthesized libraries containing more than 22 million compounds, and methods to assay up to 20 000 compounds daily are being developed. Without giving too much away, Pharmacopeia believes it can produce leads in the tens of dollars range. To get some idea of how valuable the technology is, Eli Lilly bought one company for $72 million basically to access its combinatorial chemistry abilities.

Eric M. Gordon, of Affymax, considered by many to be the most successful combinatorial chemistry company, also explained to delegates the benefits of using the small chemical molecule as the target for combinatorial chemistry. Computer-based drug design was supposed to help find new compound leads. Scientists

were supposed to create a picture of the binding site and then design molecules that bind with it. Whilst the technology clearly proved useful in optimising lead compounds it has not provided a route to create new leads *de novo*. Indeed, many companies have tended to build on existing patents thus resulting in a whole raft of me-too drugs. With health-care reforms most likely to reward innovative products only, companies need to take completely new tacks.

Affymax first started creating libraries based on peptides and oligonucleotides, and has signed up some large partners from the pharmaceutical industry to screen selected targets against these libraries. Nevertheless, it realized that peptides, owing to the problems outlined by Pharmacopeia's Baldwin, were not targets which had great appeal for the large drug companies. Affymax recruited Gordon from Bristol-Myers Squibb to add chemistry to its predominantly biological scientific staff. Gordon outlined the current state of the technology in applying encoded combinatorial library methods to drug discovery, particularly issues linked to the production of large libraries of non-polymeric organic molecules.

Bruce Seligmann, from Selectide, provided details of the Selectide process. First published in *Nature* (Vol. **345**, 84–86, 1991), by Kit Lam, the Selectide process permits the rapid synthesis of libraries of compounds and their screening either with the compounds remaining attached to solid phase particles, or following their release into solution to achieve compound concentrations of more than 20 micromoles. In the Selectide Process, the identity of the compounds is not tracked during synthesis, but instead the composition of positive compounds is determined after screening, using chemical information on the solid phase support. According to Seligmann, the medicinal chemist can custom design the libraries to improve the probability of identifying lead compounds.



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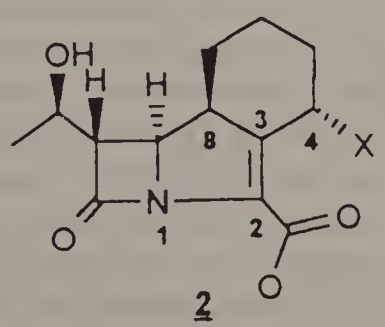


2

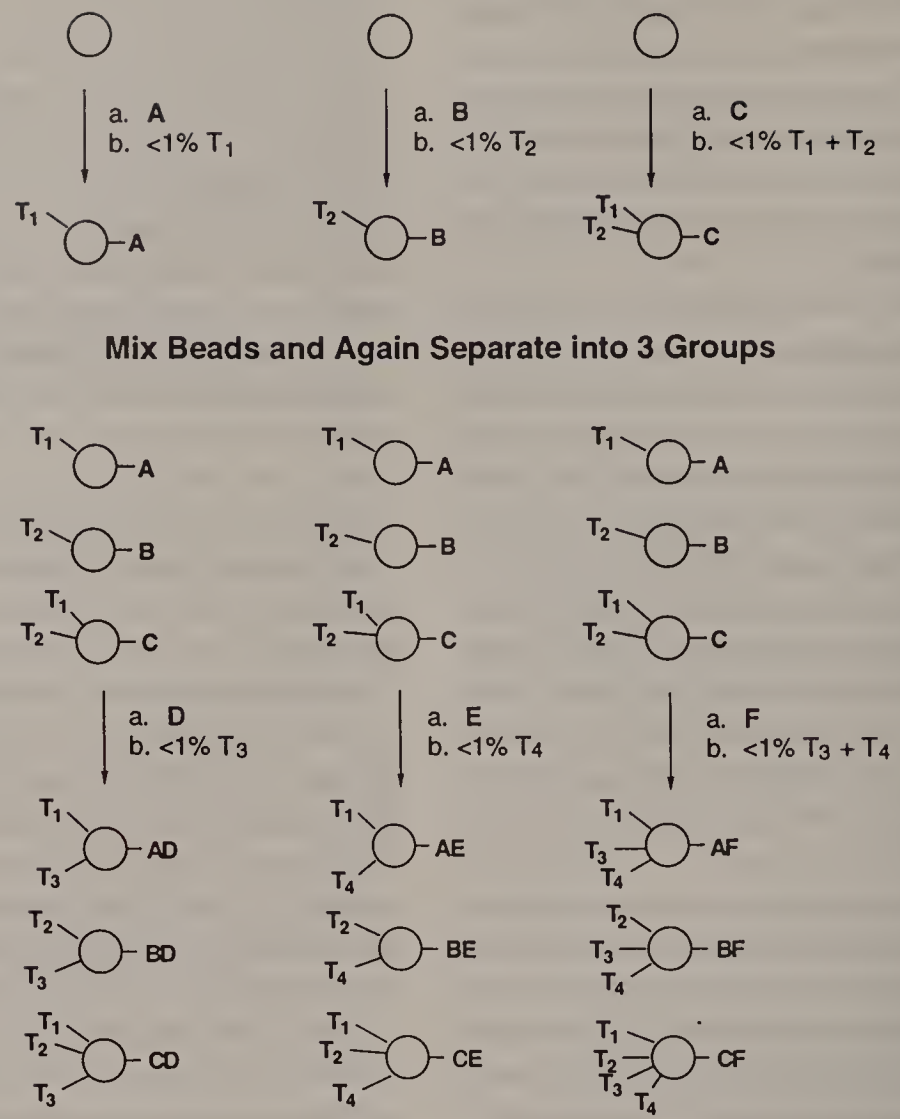
Tribactams, a new clas of β-lactam antibiotic.

Once initial leads are discovered, the method can be used to optimize the activity from micromole to nanomole by synthesising and screening secondary libraries based on the structure of the initial lead. Libraries of both peptidic and non-peptidic compounds have been synthesized and screened against both receptor and enzyme targets of pharmacological interest. Seligmann claimed that the technology has been validated by the successful identification of a Factor Xa inhibitor from libraries, and its optimization to produce compounds with sub nanomolecular *in vitro* activity. Seligmann told delegates that this is the first therapeutically relevant novel inhibitor which has been discovered and optimized from, and with, combinatorial libraries.

Whilst combinatorial chemistry is fast emerging ás a tool for drug design, the rational approach is still very popular and widely used. Bernard Roques of the Departement de Pharmacochimie Moleculaire et Structurale, Inserm, Paris, revealed the strengths of a rational approach based on target structure analogies and molecular biology studies. Genetic studies have progressed in the definition of the proteins or nucleic acid sequences to be targeted to correct deficiencies in physiological pathways, he told delegates. Details of the three dimensional arrangement of the active site of a receptor or an enzyme could serve as a basis for the design of novel molecules, which could have structures different from those of the natural ligand. Nevertheless, he pointed out, most of the examples in the clinic have been obtained by using structural analogies between protein targets and by conformational analysis of natural or screened ligands. Roques illustrated both approaches.

K. Wütrich, at the Institut für Molekularbiologie und Biophysik, E. T. H. Hönggerberg, Zürich, described the impact three dimensional structure determination of biological macromolecules by nuclear magnetic resonance in solution is having on biomedical research. Three dimensional protein structures do have key roles in biological and biomedical research; both as the basis for investigating correlations between molecular structure and physiological functions in natural systems, and as a platform for protein engineering and drug design. Although only introduced 10 years ago as a second method for protein structure determination, besides X-ray diffraction in protein crystals, about 200 n.m.r. solution structures of proteins have now been determined. Wütrich told delegates this is making an important contribution toward easing the bottleneck in rational molecular design caused by the scarcity of data on three dimensional structures.

Clearly, none of these methods has a monopolistic



30 Encoding Molecules Can Encode 2^{30} (> 1 Billion) Transformations

grip on the best way forward in drug design and many laboratories are using a combination of approaches. WC Ripka and colleagues at Corvas International (San Diego, CA) have developed effective anti-blood clotting drugs, directed at three critical enzymes of the blood coagulation cascade, using an integrated effort with molecular biology, chemical diversity, molecular modelling and drug design, and medicinal chemistry strategies. Using a molecular biology strategy of site-directed and random mutagenesis on a rigid molecular scaffold, known to be compatible with inhibition of the enzymes, their specificity requirements have been explored. These studies provided insight into the inhibitor complementary requirements of the enzyme sites and has resulted in potent, subnanomolar inhibitors of the enzymes. Ripka and colleagues have coupled this information with a mechanism-based medicinal chemistry approach to design compounds that are also effective inhibitors of the enzymes. Molecular modelling and X-ray structural information have not only confirmed the binding modes of the potential inhibitors but suggested further modifications, Ripka added.

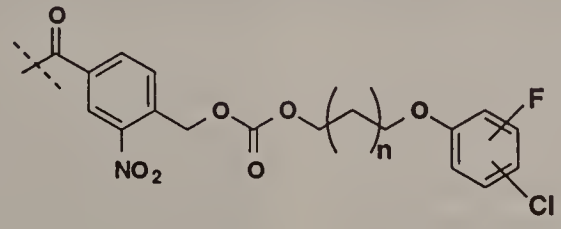
Platelet aggregation is a target for many pharmaceutical companies. Given the prevalence of heart disease in the developed world, this is hardly surprising. F. Himmelsbach at Dr Karl Thomae GmbH (Biberach, Germany) described the efforts he and his colleagues are making in the design of highly potent non-peptidic fibrinogen receptor antagonists. Many platelet aggregation inhibitors, including the world's first wonder drug aspirin, are actually quite limited in their efficacy because they tend to inhibit only one of the multiple pathways associated to platelet aggregation. The Dr Karl Thomae researchers have directed their focus on fibrinogen receptor antagonists because they suppress the final step of platelet aggregation by actually blocking the binding of fibrinogen to a glycoprotein complex on activated platelets. Himmelsbach and colleagues reported that they discovered a highly potent non-peptidic fibrinogen receptor antagonist, BIBU 52, by applying a peptidomimetic design approach. BIBU 52, and an orally active pro-drug are in phase I clinical trials. In addition, using BIBU 52 as a starting block, the researchers have designed other antagonists, such as BIBU 129, which are characterized by a cyclic urea skeleton. Moreover, Himmelsbach described how they also addressed the question of whether the benzamidino group, which has so far been a common fea-

ture of the most potent antagonists to emerge from the company, could be replaced by other basic functional groups. BIBU 251 was held up as an example of how the high potency is not restricted to benzamidines.

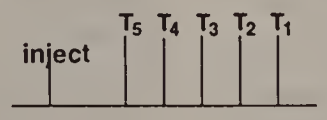
Researchers at a number of pharmaceutical companies revealed how important all these methods are in the development of new therapeutic approaches, particularly when it comes to treating previously unmet clinical needs such as human immunodeficiency virus (HIV) infection or autoimmune conditions such as multiple sclerosis. V. Kalish and colleagues at Agouron Pharmaceuticals (San Diego, CA), in collaboration with scientists at Eli Lilly (Indianapolis, IN), described iterative protein structure-based drug design and synthesis of HIV protease inhibitors. HIV protease is a key enzyme associated with the maturation of viral particles to the infectious form and, not surprisingly, has emerged as a promising target for HIV therapy. The researchers have used a two pronged approach, using protein-ligand X-ray crystal structures for iterative design, towards developing HIV protease inhibitors. One was the *de novo* design of inhibitors based on the structure of inhibited enzyme, while the second involved modular design and optimization of known inhibitors or internal leads in an iterative fashion using crystal structure information. Bother strategies, according to Kalish, have been pursued successfully and have yielded nanomolar inhibitors of HIV-1 protease. Kalish focused on candidate molecules emerging from the modular approach. One compound, designated AG1343, inhibited HIV-1 protease ($K_i = 2$ nm), displayed excellent antiviral activity ($IC_{50} = 13–60$ nm), had oral bioavailability of more than 30%, and a half life of more than 1 hour. AG1343 is now in phase I clinical trials, Kalish reported.

Bioavailability and stability are important attributes to be considered in drug design. Indeed, some of the targets for pharmaceutical researchers are not necessarily the enzymes linked to the pathology of a disease but are instead linked to enhancing the activity of a class of drugs. Beta lactam antibiotics, such as the penicillins and the cephalosporins, have had a dramatic impact on health-care provision and are amongst the best selling drugs. Many are now limited by stability or activity and the continuing spread of bacteria resistant to conventional beta lactams has created a clinical need for new compounds. G. Gaviraghi at Glaxo Research Laboratories (Verona, Italy) de-

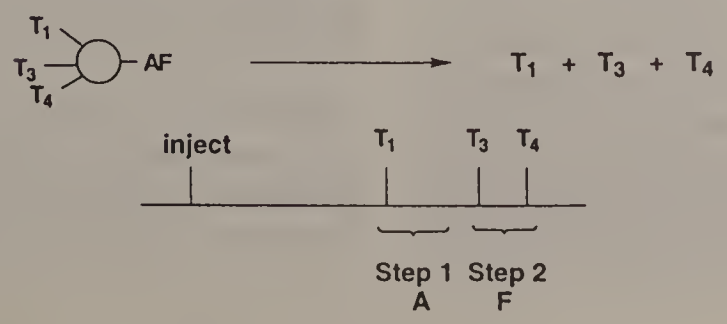
Molecular Markers are Simple, Chemically Stable Organic Molecules



Gas Chromatography with Electron Capture Detection Uniquely Identifies All Coding Molecules



Select a Bead
Detach Coding Molecules
Inject into a Gas Chromatograph to Analyze



scribed to delegates the discovery of a new class of beta lactam derivatives, called tribactams, containing a tricyclic nucleus as the key structural feature. The main characteristics of tribactams is the presence of a substituted beta lactam ring (A), an unsaturated five-membered ring (B) and a ring (C), which, in general, could be either a five-, six-, or seven-membered carbocyclic or heterocyclic ring. In particular, Gaviraghi has focused on compounds in which the (C) ring can be either unsubstituted or monosubstituted, so that the final tribactams could contain either four or five stereogenic centres. Gaviraghi told delegates that tribactams are stable to hydrolytic enzymes and possess broad spectrum antibiotic activity.

Knowledge of the metabolism in man of new pharmacologically active molecules at an early stage of research could be crucial for the choice of the best compound in a series of active molecules, D. Mansuy (Universite Paris) told delegates. Cytochrome P450 plays a key role in the metabolism of drugs in the liver. Models to mimic P450 have been developed. The first models are based on an iron porphyrin catalysts associated with an oxygen atom donor. They reproduce quite well reactions catalysed by P450 but, unfortunately, do not exhibit the substrate selectivities and oxidation regioselectivities, Mansuy explained. A new approach involving yeasts where a genetically well-defined human cytochrome P450 has been expressed in a catalytically active form has been developed. These modified yeasts can be used as simple, readily available and highly selective catalysts for predicting how each human liver P450 will metabolize a new drug, Mansuy predicted.

One of the most promising new therapeutic approaches was described by Axel Kahn of Inserm (Paris). Gene therapy, the therapeutic use of genes as drugs, has already seen some limited successes in human trials. About 80 phase I/II clinical trials in humans have been authorized around the world, some giving encouraging results. Kahn described the principles of gene therapy and explained to delegates how it can be achieved. According to Kahn, the approach will emerge as a versatile and potentially powerful type of treatment.

In addition to the 92 oral presentations, delegates to the conference also had the opportunity to study 322 poster presentations. The pharmaceutical industry was very well represented but so was Eastern Europe and Russia with 50 posters being presented by researchers based in institutes there. There were also poster presentations from researchers from PRC and Latin America.

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chem. Intl.* as recent reports.

If you would like to comment on the Provisional Recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat.

Photochemistry

The Commission on Photochemistry (III.3) of the Organic Chemistry Division has produced a Glossary of Terms used in Photochemistry. This is in fact the second edition and has been prepared by Jan W. Verhoeven, Amsterdam, the Netherlands. The glossary is arranged in alphabetical order, beginning with Absorbance (A) and ending with Zero–Zero (0–0) Absorption or Emission. Each term is explained in some detail with numerous cross references. For example, under Photon exposure (H_p) one is referred to the sections on fluence and radiant exposure. The final section of the report is a very useful definition of symbols and units. The units are given in both SI and more familiar, or common, form. Apart from definitions and explanations, this glossary also contains notes on different types of lasers and on various chemical reactions, including photoinduced electron transfer processes.

In this second edition, a number of minor errors encountered in the first edition have been corrected and it has been expanded to include additional terms.

It is hoped that this revised and expanded glossary will continue to serve its purpose, which is to provide definitions of terms and symbols commonly encountered in the field of photochemistry in order to achieve consensus on the adoption of some definitions and on the abandonment of inadequate terms.

Comments on these recommendations are welcome and should be sent by 30 June 1995 to: Dr J. D. Coyle, Cookson Group plc., Cookson Technology Centre, Sandy Lane, Yarnton, Oxon. OX5 1PF, UK.

Photorefractive Polymers

The photorefractive effect was first observed as an unwanted deterioration in the optical quality of certain inorganic crystals used inside optically pumped laser resonators. Indeed, it was for many years an inexplicable and expensive problem. It is now, however, recognized as a promising way of producing holograms and consequently as a means of storing and retrieving data at high repetition rates.

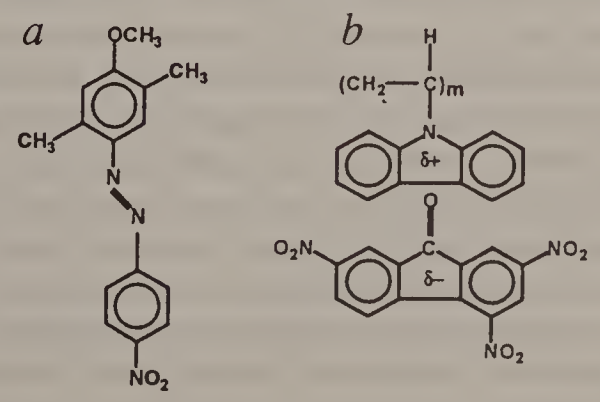
The ability to store and retrieve data easily and rapidly in solid materials is one of the limiting steps in new generations of information technology. Holographic optical storage is one of the most promising of current ideas. A system based on writing and reading multiple holograms in the same volume of material offers high storage density. If two dimensional laser arrays could be used to write the information, then the use of charged coupled devices to read the information offers particularly rapid rates of data transfer.

When two light (laser) beams intersect and are incident upon a material capable of displaying a photorefractive response, an interference pattern in created with a strongly nonuniform distribution of light intensity. At those points exposed to intense illumination there will be optical absorption, possibly at charge transfer bands, producing an intrinsic charge separation within the solid. If these charges are distinctly localized on particular parts of the molecules being illuminated, at distinct chromophores, there will be further charge separation which may well persist after illumination has ceased and a local electric field will be generated at the molecular level due to the induced electric dipoles (charge separation multiplied by distance). This induced electric field will follow the same intensity modulation as the interference pattern of the incident light beams. For a material to be photorefractive it must possess a local refractive index which is dependent upon the local electric field, and, indeed, it must vary linearly as the local electric field varies. That is, it must possess a crystal structure with an asymmetrical unit cell as is the case for materials which frequency double. In this way a refractive index grating is established, this refractive index grating being a hologram which can diffract light.

Until quite recently, the only materials which were thought to display the photorefractive effect were inorganic crystals, e.g. $LiNbO_3$, and early work showed the potential for such materials in optical processing, holographic technology, phase conjugation and data storage. However, their use has been limited due to the cost of growing sufficiently large perfect crystals of these low symmetry materials.

Polymers capable of displaying a photorefractive response have many advantages over inorganic photorefractive crystals, lower dielectric constant, lower cost, ease of fabrication and structural flexibility. K. Meerholz and colleagues from the Optical Sciences Centre, University of Arizona, USA, and scientists from IPCMS, Groupe d'Optique Nonlinéare et d'Optoélectronique, CNRS, Strasbourg, France, have recently reported (*Nature* **371**, 497–500 (1994)) a particularly effective photorefractive polymer, to be exact it is a polymer composite. Their investigations were based on the photoconductor poly(*N*-vinylcarbazole) (PVK), photosensitivity in the visible was achieved by adding 2,4,7-trinitro-9-fluorenone which forms a charge transfer composite complex with the PVK. The electro-optic chromophore, which must be soluble in this composite, and have a large electric dipole moment together with a very anisotropic electric polarizability was 2,5-dimethyl-4-(*p*-nitrophenylazo)anisole. The appropriate low symmetry of the final solid state unit cell, necessary to obtain a macroscopic electro-optic effect, was produced by forming the solid from solution in the presence of an intense laboratory applied static electric field. In this way the molecules are oriented as they assemble into the solid.

Future work on this type of low-cost electro-optic polymer system are likely to have a profound effect on developments in information technology.



Chemical structures of the compounds used in the photorefractive composite: (a) 2,5-dimethyl-4-(*p*-nitrophenylazo)anisole (DMNPAA); (b) charge-transfer complex of poly(*N*-vinylcarbazole) (PVK) with 2,4,7-trinitro-9-fluorenone (TNF).

Recent Reports

Impedances of electrochemical systems: Terminology, nomenclature and representation – Part I: Cells with metal electrodes and liquid solutions (IUPAC Recommendations 1994)

This document provides an inventory of the parameters used to describe impedances of electrochemical cells, in particular, those consisting of metal electrodes and solution electrolytes. The method of impedance measurements is widely used in many fields of electrochemistry, for example, electrode kinetics, batteries, corrosion studies and bioelectochemistry (membranes). It is a linear response method, in that the system is perturbed by modulation of small amplitude and the measured response contains only first order terms. The definitions of these parameters are given, as well as recommendations for their terminology and nomenclature. Where relevant, experimental determination of a parameter and limitations to its validity are briefly discussed. Also considered are inhomogeneities, including porosity, of the electrode surfaces.

This report was prepared for publication by M. Sluyters-Rehbach, Electrochemistry Department, Utrecht University, the Netherlands; and Commission on Electrochemistry of the Physical Chemistry Division. The details are published in Pure Appl. Chem. ***66****, 1831–1891 (1994).*

Nomenclature and terminology of graphite inclusion compounds (IUPAC Recommendations 1994)

Recommendations are presented for the nomenclature and terminology of graphite intercalation compounds, that is, compounds that retain the planarity of the carbon layer in the graphite structure. Not included are those compounds with covalent bonding between the carbon atoms and the intercalated heteroatom which leads to sp^3 hybridization of the carbon atoms and the corresponding lose of planarity. Rules for a structural notation, including multiple intercalation materials, are described in addition to those for the naming and the formulation of graphite intercalation compounds.

This report was prepared for publication by Hanns-Peter Boehm (Institut für Anorganische Chemie der Universität, D-80333 München, Germany), Ralph Setton (Centre de Recherches sur les Solides à Organization Cristalline Imparfaite, F-45071 Orléans, France) and Eberhard Stumpp (Institut für Anorganische Chemie der Universität Clausthal, D-38678 Clausthal-Zellerfeld, Germany); and the Commission on High Temperature and Solid State Chemistry of the Inorganic Chemistry Division. The details are published in Pure Appl. Chem. ***66****, 1893–1901 (1994).*

Nomenclature of interlaboratory analytical studies (IUPAC Recommendations 1994)

Three major types of interlaboratory analytical studies, in which a group of laboratories analyse identical test portions from a homogeneous test sample, are defined and discussed. Each type is characterized by an appropriate designation. (1) Method-performance study – A study in which all laboratories follow the same written protocol and use the same test method to measure a particular property. Thereby testing performance parameters of a particular method. (2) Laboratory performance study – A study where each laboratory uses the method of their choice in order to assess the performance of that laboratory. (3) Material certification study – A study that assigns a reference value to a characteristic in the test material, usually with a stated uncertainty, using the best laboratories and the least-biased method.

This report was prepared for publication by William Horwitz, Centre for Food Safety and Applied Nutrition, Food and Drug Administration, Washington, DC 20204, USA; and the Commission on Analytical Nomenclature and the Commission on General Aspects of Analytical Chemistry of the Analytical Chemistry Division. The details are published in Pure Appl. Chem. ***66****, 1903–1911 (1994).*

Analytical techniques for trace organic compounds – VI. Application of liquid chromatography-mass spectrometry (Technical Report)

The combination of liquid chromatography and mass spectrometry, where the mass spectrometer is used as a very sensitive means of detecting the eluted molecules, is becoming increasingly common. Such facilities are now routinely used for a wide variety of samples. The most successful device appears to be the atmospheric pressure source with electrospray and chemical ionization. This report details some of the advantages and disadvantages of different experi-

mental set-ups and attempts to give some relative sensitivities. Furthermore, criteria are indicated which may be applied when a choice has to be made on the basis of analytical requirements, technical and financial considerations.

This report was prepared for publication by, Michael Linscheid (ISAS Institut für Spektrochemie, D-44139 Dortmund, Germany) and David G. Westmoreland (Rohm and Haas Company, 727 Norristown Road, Spring House, PA, USA); and the Commission on Microchemical Techniques and Trace Analysis of the Analytical Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 1913–1930 (1994).*

Structure–activity relationships for biodegradation: a critical review (Technical Report)

Although of considerable interest, there is a paucity of experimental data concerning the environmental fate of organic chemicals. This has necessitated the development of a number of theoretical models, based solely on the chemical structure and physico-chemical properties of the molecules concerned, to investigate these environmental processes. With the aim of assessing the limitations of such Quantitative Structure Biodegradation Relationships (QSBRs) presently available, this report reviews the approaches used to derive QSBRs and the results obtained with various models. Also, some aspects of the integrated approach that needs to be followed in order to be able to predict real biodegradation rates in soil and water are presented.

This report was prepared for publication by W.J.G.M. Peijnenburg, National Institute of Public Health & Environmental Protection, Laboratory for Ecotoxicology, 3720 BA Bilthoven, the Netherlands; and the Commission on Water Chemistry of the Applied Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 1931–1941 (1994).*

PAC Review

Pure and Applied Chemistry (*PAC*) is IUPAC's official journal. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in *PAC* are published in *Chem. Intl.* in the section Recent Reports. In this section we take a brief look at the symposia and lectures published in recent issues of *PAC*.

High temperature material chemistry

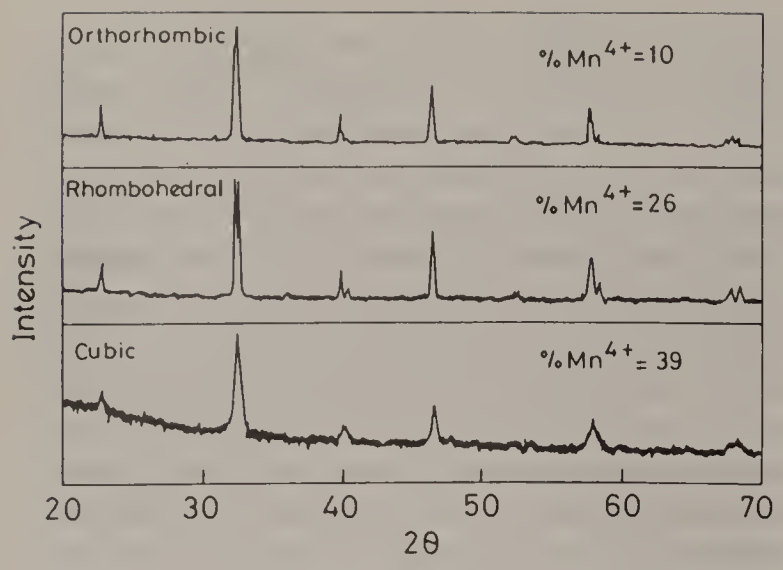
The September 1994 issue of *Pure Appl. Chem.* contained the nine plenary lectures presented at the 8th International Conference on High Temperature Materials Chemistry (HTMC VIII) held in Vienna, Austria, 4–9 April 1994.

This meeting was supported by the Physical and Inorganic Chemistry Divisions and the Co-ordinating Committee on Chemistry and Advanced Materials Programme in conjuction with University of Vienna, Technical University of Vienna and the Gesellschaft Österreichischer Chemiker. The conference editor was Professor A. Mikula (Institute of Inorganic Chemistry, University of Vienna, Währingerstrasse 42, A-1090 Vienna, Austria).

The main topics of the conference were: Advanced materials for high temperature applications, New ceramic materials, Thermodynamics and kinetics at high temperatures, Modelling and data bases, New measurement techniques and Materials under extreme environmental conditions.

The plenary lectures presented an interesting overview of the state-of-the-art in high temperature ceramics, a subject which has particular relevance to the current interest in the development of ceramic high temperature superconductors. Other invited lectures covered another area of material science which is currently receiving considerable attention, that of diamond fabrication and diamond film formation on suitable substrates.

Alexander Navrotsky (Princeton Materials Institute and Department of Geological and Geophysical Sciences, Princeton University, NJ 08544, USA) discussed the thermodynamics of the formation of Perovskite-related oxides with high oxidation states, i.e. materials used in high temperature superconductors, electrochemical sensors and solid oxide fuel cell electrodes. The experimental measurements consisted of high temperature reaction calorimetry, that is, measuring the enthalpy of formation of these oxides in the presence of various additional ions. For example, it was found that the enthalpy of formation from the oxides of a series of ternary oxides containing formal Cu^{3+} becomes increasingly exothermic with decreasing



Rhombohedral and cubic $LaMn^{3+}Mn_x^{4+}O_{3+\delta}$ obtained by the electrochemical oxidation of orthorhombic $LaMnO_3$.

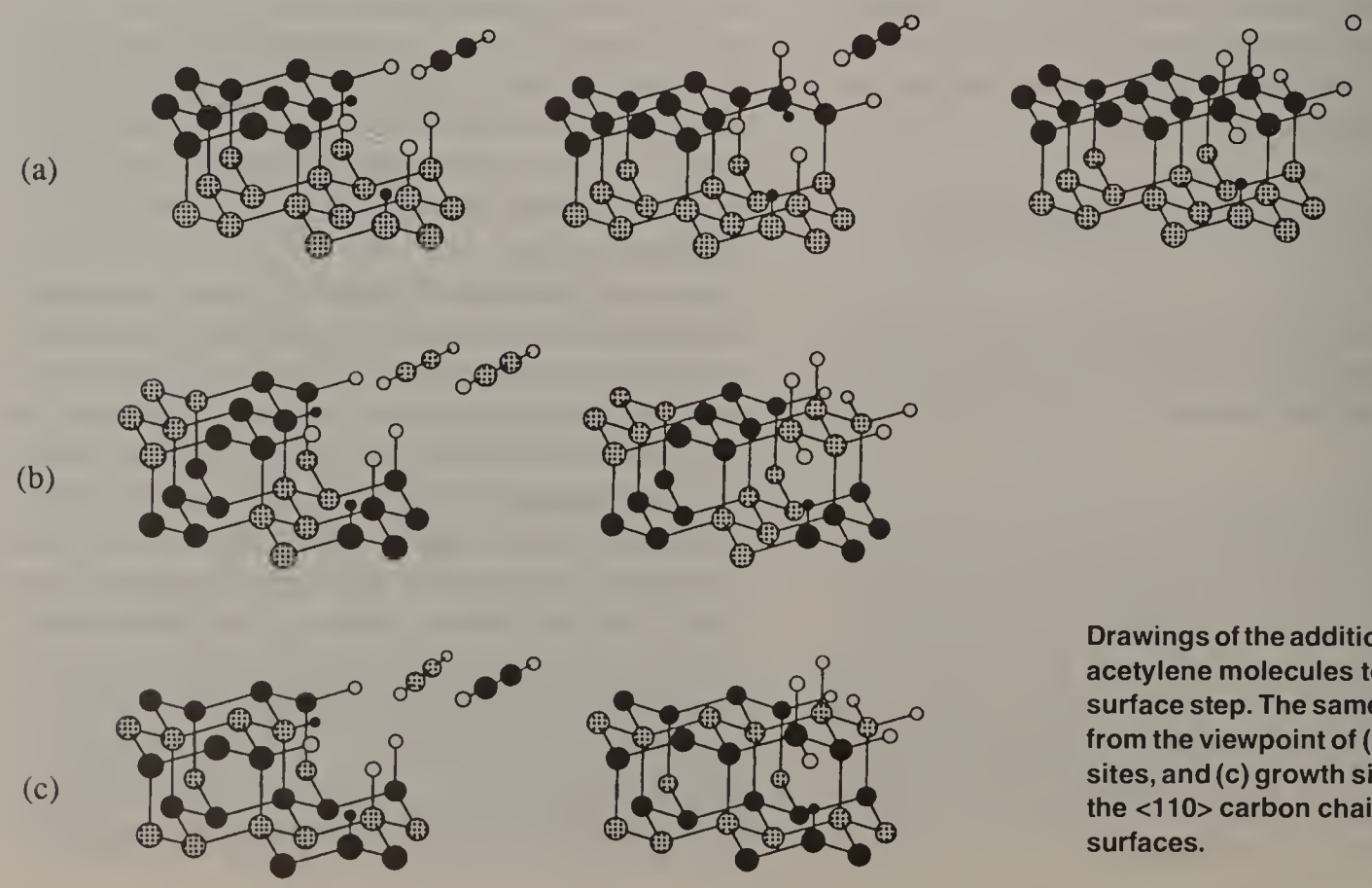
ionic potential, i.e. charge to size ratio, of the counterbalancing cation in the series $LaCuO_3$, $LaSrCuO_4$, $LaBaCuO_4$, $NaCuO_2$ and $KCuO_2$. All these components are found in the structures of the different classes of ceramic high temperature superconductors. Of great interest to synthetic solid state chemists was the observation that the overall energetics of such reactions are governed by the competition of oxygen vacancy formation, oxidation to formal M^{3+}, and coupled ionic substitution. Energetic parameters for these defect formation reactions were derived from the measured calorimetic data.

C. N. R. Rao (Solid State & Structural Chemistry Unit and CSIR Centre of Excellence in Chemistry, Indian Institute of Science, Bangalore 560012, India) a past President of IUPAC, gave an overview of the various chemical approaches to the design of oxide materials, where considerable chemical ingenuity is required in the synthesis of solid materials. Tailor-making materials of the desired structure and properties, for example, a high temperature superconductor with a particular transition temperature to the superconducting phase, is one of the main goals of material chemistry, but it is not always possible to do so with conventional methods. Rational design has indeed provided a wide variety of materials, the large number of porous and microporous, zeolite-like, materials being typical examples. However, such rational design approaches generally give thermodynamically stable materials, but may miss new and interesting metastable structures. Professor Rao showed how mild or soft chemical routes, such as electrochemical deposition, could be used to synthesis materials which had previously only been made by high temperature methods.

Understanding the high temperature chemistry of diamond synthesis and deposition is a key to turning recently developed chemical vapour deposition techniques into useful technological applications. Karl E. Spear and Michael Frenklach (Materials Science and Engineering Department, The Pennsylvania State University, University Park, PA 16802, USA) have investigated the chemical mechanism of chemical vapour deposition growth of diamond coatings made from carbon-hydrogen systems reacting at, for example, a graphitic substrate surface at high temperature, that is

$$CH_4(g) \text{ activated} \rightarrow C(\text{diamond}) + 2H_2(g)$$

The authors present mechanisms which explain how, for example, CH_3 molecules may be incorporated into a monolayer covering and how diamond-like (sp^3 hybridized) carbon lattices form. Other authors at the conference presented results on other types of substrates.



Drawings of the addition of two acetylene molecules to (a) a {111} surface step. The same additions, but from the viewpoint of (b) {110} surface sites, and (c) growth sites extending the <110> carbon chains in a {100} surfaces.

Chemistry of natural products

The October and November issues of *Pure Appl. Chem.* for 1994 have been combined into a single volume which contains details of the 19th International Symposium on the Chemistry of Natural Products held in Karachi, Pakistan, on 16–20 January 1994. The meeting was organized by the Organic Chemistry Division in conjuction with the H. E. J. research Institute of Chemistry of the Chemical Society of Pakistan. The Symposium Editor was Atta-ur-Rahman (H. E. J. Research Institute of Chemistry, University of Karachi, Karachi 75270, Pakistan).

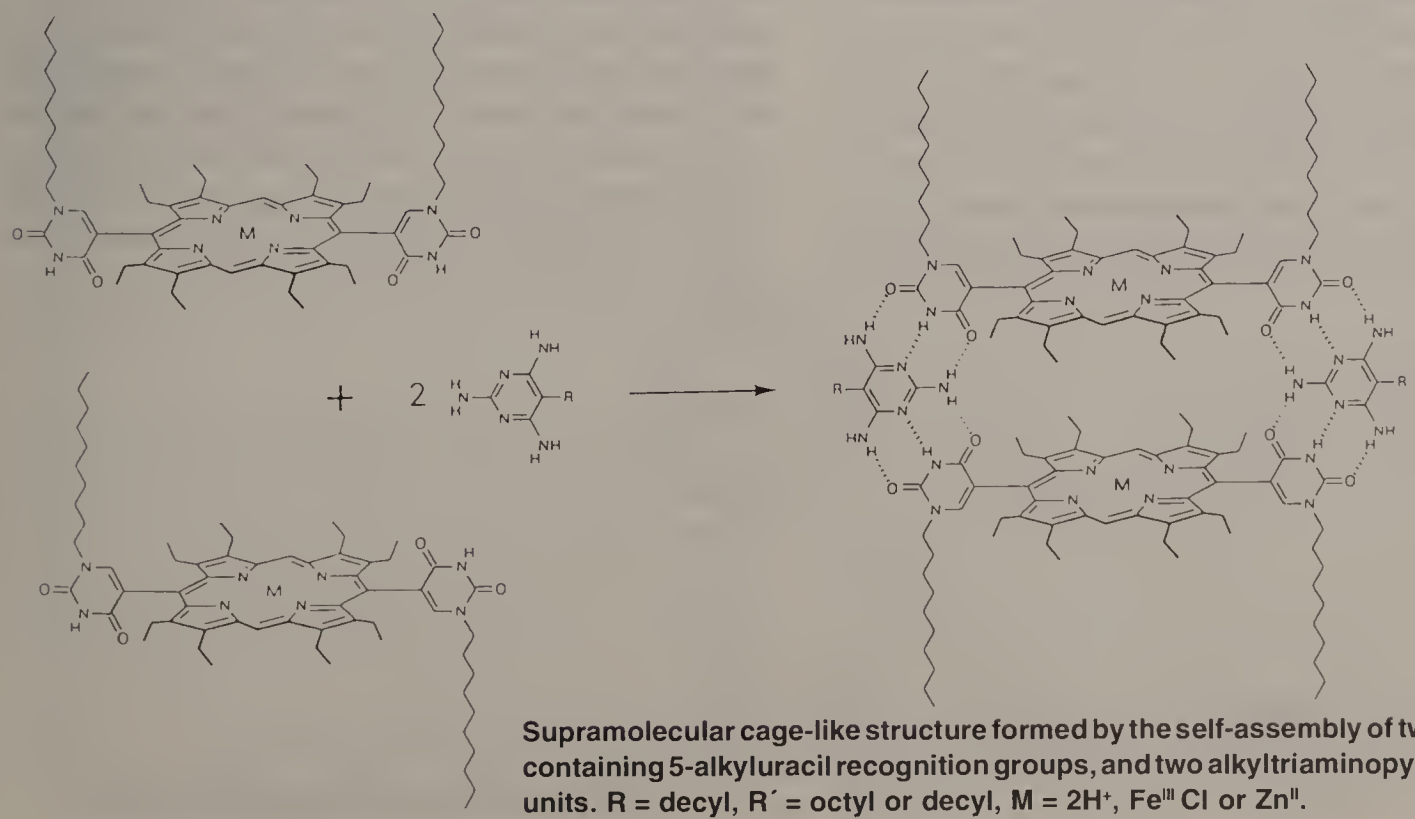
Natural product chemistry is at present experiencing something of a *renaissance*. This has been brought about by recent rapid advances in the field of stereoselective methods in organic synthesis (for a recent contribution to this newly expanding literature see Publications section in this issue). New sophisticated techniques for the separation and identification of bioactive natural products, and the integration of the bioassay techniques with the isolation procedure have reinvigorated this field.

The present Symposium contained stimulating accounts of recent investigations of the chemistry of many important, interesting and complex natural products. The articles presented at this symposium included the total synthesis of a large number of natural molecules; the isolation and structure elucidation of bioactive natural products from terrestrial, marine and microbial sources, biosynthesis of natural molecules, together with recent developments in spectroscopic techniques for the structure elucidation of natural products.

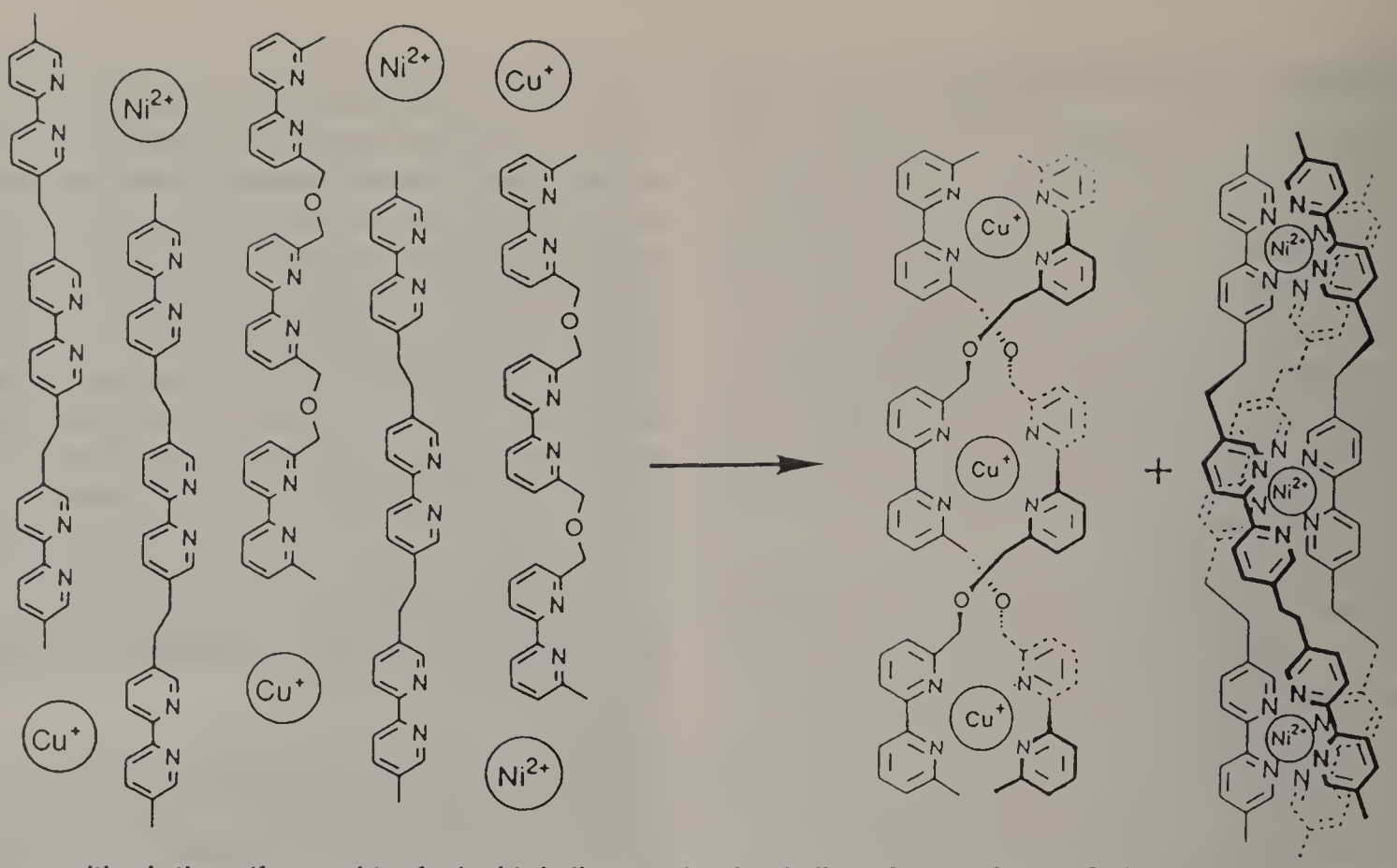
There were three special lecture each given by a Nobel Laureate, D. H. Barton (Department of Chemistry, Texas A&M University, College Station, TX 77843, USA) spoke about the invention and design of chemical reactions of relevance to the chemistry of natural products. How new reagents and reactions, for use in natural product chemistry, can and should be invented not just discovered by chance. That is, one should adopt a systematic approach to the synthesis of very complex molecules. We must recognize that a reaction can be important synthetically, but which does not yet exist in a satisfactory form. Thus the reaction of interest either does not exist, or if it does, it is carried out under extreme conditions without any selectivity. Poor yields, uneconomic reagents and lack of stereo-selectivity are other factors that spur invention. Professor Barton's talk demonstrated elegant multiple step syntheses, but with high yield, of many complex molecules of biological significance, for example, a phosphate analogue of AZT the main anti-AIDS drug.

Professor Richard E. Ernst (Laboratorium für Physikalische Chemie, Technische Hochschule, 8092 Zürich, Switzerland), who won the Nobel Prize for his work on Nuclear Magnetic Resonance (NMR) spectroscopy, spoke about the use of NMR to study the intramolecular dynamics of large molecules. This is an area of great current interest, it was previously only possible to determine the structure of large molecules, for example, protein molecules, using x-ray or neutron diffraction, however, such is the power of modern NMR spectroscopy that it is now possible to directly study the conformational dynamics and motions of large molecules in solution. Such measurements go a long way to establishing the tertiary structure of complex biological molecules under natural conditions. Consequently, it is not now necessary to grow large single crystals to elucidate structure, the dynamics can be studied under natural conditions.

The third Nobel lecturer was Jean-Marie Lehn (Université Louis Pasteur, 4 rue Blaise Pascal, 67000



Supramolecular cage-like structure formed by the self-assembly of two porphyrins, containing 5-alkyluracil recognition groups, and two alkyltriaminopyrimidine (TAP) units. R = decyl, R´ = octyl or decyl, M = $2H^+$, $Fe^{III}Cl$ or Zn^{II}.



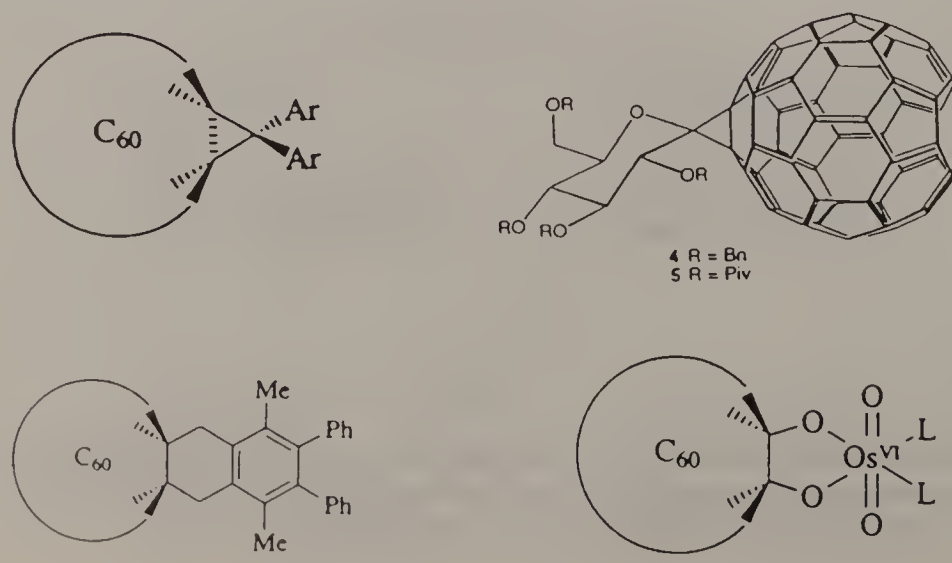
Self-recognition in the self-assembly of a double helicate and a triple helicate from a mixture of oligobipyridine strands and of Cu^{I} and Ni^{II} ions (ClO_4 – anions omitted).

Strasbourg, France and Collège de France, Paris) who spoke about molecular self-assembly. How molecules can recognize each other and spontaneously assemble into large scale structures held together, for example, by hydrogen bonding; Supramolecular Chemistry.

One of the many studies of synthetic routes to important natural products given at this symposium was an investigation of the biosynthesis of *taxol* by P. E. Fleming *et al.* (University of Washington, Seattle, WA 98195, USA). Due to its mode of action and promising early clinical trials, *taxol* commands considerable interest as a new naturally occurring anticancer agent. However, the complexity of its structure presents a considerable challenge to synthetic organic chemists and naturally raises the question of how the plant assembles this complex molecule. The present studies have used strategically labelled radioactive precursors to investigate the biosynthesis of this important molecule.

There continues to be considerable interest in C_{60} (Buckminsterfullerene). Harold Kroto *et al.* (University of Sussex, Brighton, UK) have been investigating the chemical reactivity of this new form of carbon. C_{60} contains 30 double bonds endocyclic to the 20 adjacent hexagons and exocyclic to the 12 isolated pentagons which comprise the highly symmetrical icosohedral structure. As a result the cage exhibits chemical properties commensurate with those of an electron-deficient polyene.

As is well known, the addition of a second substituent onto a previously substituted benzene molecule is strongly influenced by the nature, of the first substituent (electron giving or electron pulling), and the location, relative to the site of the second addition, of the first side group. What happens, however, when one deals with a much larger aromatic system – C_{60}? What are the equivalent rules governing *ortho, meta* and *para* substitution, and activation and deactivation of the electronic structure, in a much more de localized aromatic molecule? The work of Kroto *et al.* is attempting to unravel these interesting questions.



Recently made compounds involving C_{60}.

Publications

Solubility Data Series, Vol. 56. Alcohols with Hydrocarbons

Oxford University Press (OUP) has published this, the most recent volume of the Solubility Data Series. Volume 56 contains a compilation of precision data on the solubility and phase diagrams for hydrocarbons and alcohols. Solubilities at elevated and lowered temperatures and at variable pressure have been included.

For some systems, the two components may be miscible in all proportions at certain temperatures and pressures. Data on reported miscibility gaps together with upper and lower critical solution temperatures are included where appropriate and when available.

Data are presented in two forms; tables of the original experimental values obtained from a critical reading of the literature, and a recommended value. Also included are discussions concerning the criteria used in selecting and rejecting data which has subsequently been fitted to simple model curves.

The IUPAC Solubility Data Series, ISSN 0191-5622, is published quarterly by OUP. Subscription is USD395 a year. Enquiries should be addressed to OUP, 2001 Evans Road, Cary, NC 27513, USA (USA and Canada enquiries only), or Journals Customer Services, OUP, Walton Street, Oxford OX2 6DP, UK

Stereocontrolled organic synthesis

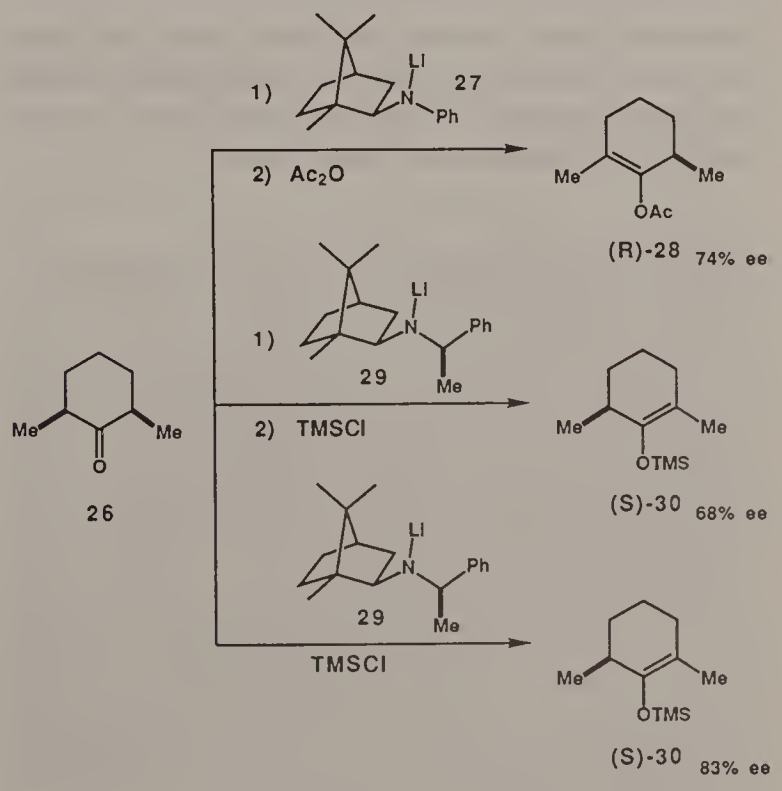
As any professional chemist will tell you, synthesis is at the very core of chemistry. The formation of new substances and materials is vital to meet the continuing, and ever changing needs of our society. Nearly every aspect of daily life, from food to communications, requires novel and more advanced materials with evolving properties. It is the chemist who must respond to these ever changing demands and develop, through novel synthetic pathways, new more versatile materials.

As in most interconnected research endeavours, synthetic chemistry develops from advances that arise in other branches of chemistry. For example, new advances in theoretical and mechanistic chemistry prompt experimental chemists to test and advance these ideas, and to broaden the scope and power of existing reactions.

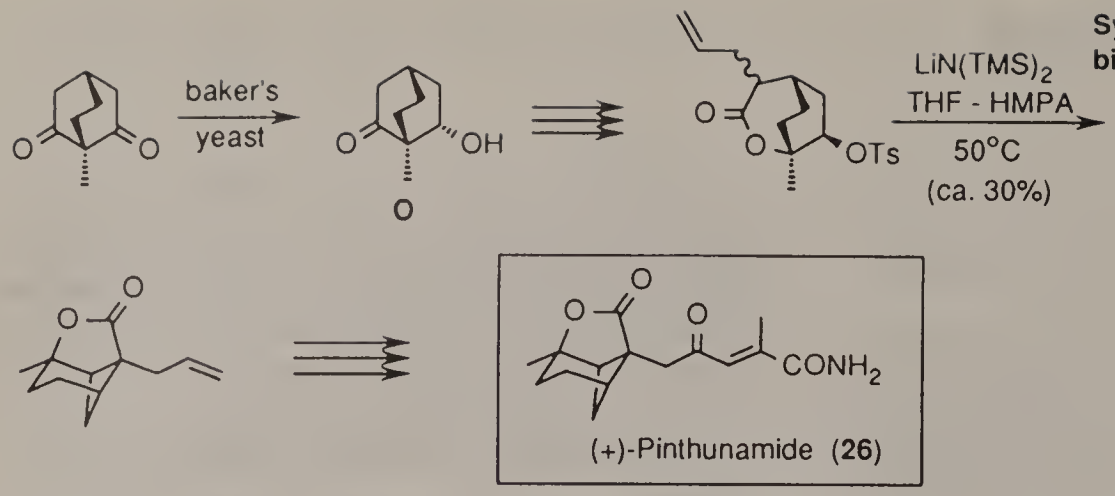
One could say that the goal of synthetic chemistry is efficiency, we seek the shortest possible route from inexpensive, readily available starting materials to the desired, precious target molecule. The interplay of synthetic strategy and synthetic methods provides the mechanism to achieve this goal. Earlier in this issue of *Chem. Intl.* there is a report on the 19th International Symposium on the Chemistry of Natural Products held in Karachi, Pakistan, where many of these ideas were discussed.

Selectivity continues to be one of the main themes in the development of new synthetic routes. Nature provides abundant examples, and indeed sources, of new molecules, however, these molecules are produced by naturally stereoselective methods. If the synthetic chemist is to make use of these starting materials then he must have similarly powerful stereoselective synthetic pathways.

Solutions to the problems of enantioselectivity rely largely upon either resolution methods or the availability of pure enantiomers of the starting material. In this present volume, the chapters by Noyori, Narasaka and Mukaiyama and Kobayashi reveal some of the efforts to use abiological catalysis to resolve this problem. After a century of stoichiometric organometallic chemistry, Reetz shows how we may affect the stereochemistry and regioselectivity of a reaction involving optically active organometallic compounds by modifying the metal environment. The chapter by Otera *et al.* explores the use of heteroatoms for similarly adjusting stereoselective reactivity. The power of stoichiometric



Use of a monodentate chiral lithium amide in different experimental conditions to control chirality of reaction products.



Synthesis of (+)-pinthunamide using a biologically derived starting material.

stereochemical control elements and how practical solutions may be derived from them are discussed by Meyers and Posner.

Developing synthetic equivalents for existing reactions may prove a useful technique in controlling stereochemistry. Designing organometallic reagents as enolate equivalents is discussed by Thomas and Hoffmann. This work clearly displays the inter-relationship between synthetic methods and synthetic strategy. Other topics covered include the merging of the field of biology and chemistry as evidenced by the increasing use of biological methods in chemical synthesis. Indeed, being a vibrant field of study, synthetic chemistry has become sufficiently powerful as to become a technology for probing biological phenomena.

This volume has been issued as one of the IUPAC monographs on Chemistry for the 21st Century. To live up to this title is quite a daunting task for any author, however, the synthetic chemistry displayed here is right at the cutting edge of research and will certainly be of use in the approaching new century.

Stereocontrolled Organic Synthesis *was edited by Barry M. Trost and published by Blackwell Scientific Publications, 1994. x + 482 pp. ISBN 0865 42833 6 (Hardback). Price: GBP70.00/USD99.50.*

Locally Produced Low Cost Equipment for the Teaching of Chemistry

The Locally Produced Low Cost Equipment (LPLCE) programme is CTC's major success. The thought which lies behind it is elegant in its simplicity. In underdeveloped countries, for educational purposes, commercial instruments and apparatus are often too expensive and too complicated to use. Moreover, such equipment may be troublesome to maintain and to repair, requiring an expensive and hard-to-find servicing department. Indeed, the measurements derived from commercial instruments may well be too detailed and precise for educational purposes.

Now that we can work with readily available transistors and integrated circuits, it is far more sensible to build such equipment and instruments, that may be needed, ourselves. Building your own equipment in this way has several advantages: (i) the cost of home-made apparatus is a fraction of what one would pay for commercial equipment; (ii) the teacher-constructor knows how it was built and therefore how to handle it; (iii) in case of a breakdown it can readily be repaired. It has to be said in passing that home-made instruments are often more robust than factory produced ones. That they are less accurate than commercially available instruments is not necessarily a problem for educational purposes. However, at present the accuracy can come remarkably close to commercial standards, and the home-made instruments are beginning to look more professional.

This monograph describes the fabrication, use and maintenance of three instruments, a pH meter, a conductometer and a colorimeter, having widespread use in the teaching of laboratory based chemistry courses. Also described are the fabrication of two test instruments, a continuity tester and an OVA source, which are useful instruments for trouble shooting and for calibration; and of several accessories such as magnetic stirrers, a zero-cost electrode for pH measurement and a conductance cell.

Brief theoretical sections in chemistry and electronics are included to make this monograph self contained. No previous experience in instrument fabrication is assumed; practical techniques such as soldering, PCB manufacture and circuit board assembly are therefore described in some detail. The monograph is liberally illustrated and uses a highly visual style of description where frequent reference is make to the accompanying illustrations.

The equipment described has been developed under the project on Low Cost Equipment for Chemical Education sponsored first by the Committee on the Teaching of Chemistry of IUPAC and UNESCO and subsequently by the DST and by UGC. Valuable assistance has also been received from IDRC, ICSU CTS and from the Commonwealth Foundation. The immediate aim of the project is to develop teaching-oriented instruments for chemistry which are simple, reliable, inexpensive, easy to fabricate and easy to maintain. A wider aim is to influence laboratory teaching by making

it more purposeful, exciting and innovative. The experience developed under the project is therefore being disseminated through practical teacher training workshops. Twenty five such teacher training workshops have been held outside India under the auspices of UNESCO while 35 workshops have been organized in India under the sponsorship of UGC.

The kits/equipment described in this monograph are manufactured, under a DST license, by the Low Cost Teaching Aid Charitable Society, 389/7 Dikhush Bagh, G.T. Karnal Road, Delhi-110033, India.

Locally produced Low Cost Equipment For The Teaching Of Chemistry by K.V. Sané and D. C. West. Printed and Published by Shatabdi Computers Pvt. Ltd, Delhi, India.

Fluorides and Oral Health

Fluoride, in particular in toothpaste and drinking water, is widely used throughout the world to prevent dental caries. There is clear evidence that regular, low-level exposure of a population to fluoride can reduce caries prevalence. However, the most cost effective way of delivering the fluoride depends on available resources, the caries status with the community, and existing environmental sources of fluoride exposure.

One of the Expert Committee of the World Health Organization has produced a short booklet on the subject of fluoride and dental health. They make recommendations which are designed at promoting increased use of fluoride within developing countries.

The WHO Technical Report Series makes available the findings of various international groups of experts that provide WHO with the latest scientific and technical advice on a broad range of medical and public health subjects. ISBN 92-4-120846-5, 37 pages, CHF8 in developed countries and CHF5.6 in developing countries. Further information and copies are available from, Distribution and Sales, World Health Organization, 1211 Geneva 27, Switzerland.

Environmental Health Criteria

The Environmental Health Criteria (EHC) monographs produced by the International Programme on Chemical Safety include an assessment of the effects on the environment and on human health of exposure to a chemical or combination of chemicals, or physical or biological agents. They also provide guidelines for setting exposure limits.

The purpose of a Health and Safety Guide (HSG) is to facilitate the application of these guidelines in national chemical safety programs. The first three sections in a HSG highlight the relevant technical information in the corresponding EHC. Section 4 deals with advice on preventive and protective measures and emergency action; health workers should be thoroughly familiar with the type of information found in this section. The section on regulatory information has been extracted from the legal file of the International Register of Potentially Toxic Chemicals (IRPTC) and from other United Nations sources.

Three new guides have recently been published, they are:

- Health and Safety Guide No. 86, *Methyl Bromide* (ISBN 92 4151086 2);
- Health and Safety Guide No. 87, *Chloroform* (ISBN 92 4151087 0);
- Health and Safety Guide No. 88, *Phenol* (ISBN 92 4151088 9).

Published by the World Health Organization for the International Programme on Chemical Safety. These publications are priced CHF5 in developed countries and CHF3.5 in developing countries. Further information and copies are available from, Distribution and Sales, World Health Organization, 1211 Geneva 27, Switzerland.

Cationic Polymerization and Related Ionic Processes

The August issue of *Die Makromolekulare Chemie: Macromolecular Symposium* (Vol. **85**, 1–392) publishes many of the key papers presented at the 11th International Symposium on Cationic Polymerization and Related Ionic Processes, which was organized under the auspices of IUPAC and the Institute of Polymers of the Bulgarian Academy of Sciences, held at the Borovets resort, Bulgaria, July 1993. The symposium was attended by 111 scientists from 22 countries. The scientific programme of the Symposium included 27 main lectures, 14 oral communications and 24 poster communications from the field of cationic and anionic polymerizations.

The main topics of the discussion included: the nature of the active centres in ionic polymerization and the influence of additives (electron donors, electron acceptors and salts) on polymer chain growth; tailor-made polymers and co-polymers with definite structure and composition; new methods for functionalization of polymers; the application of polymeric materials prepared by ionic polymerization.

The Symposium was sponsored by the Bulgarian Academy of Sciences, the National Science Foundation of USA, Technological University, Bourgas, the Neftochim company, Bourgas, the Neochim company, Dimitrovgrad, the Bank for Economic Projects 'Mineralbank', Sofia, and Engineering Plastics Evstatiev, Sofia.

Method	*Counteranion*	*Added Base*	*Added Salt*
Activator	I_2, ZnX_2, SnX_2, $Zn(acac)_2$	$EtAlCl_2$, $SnCl_4$	$SnCl_4$, $TiCl_4$
Initiator	HX (X = I, Br, Cl) R-COH (=O) R-⟨⟩-COH (=O) CH_3SO_3H $(RO)_2$-POH (=O) CH_3-CH(OR)-X (X = OAc, Cl)	HCl R-COH (=O) (R = CF_3, CH_3) CH_3-CH(OR)-X (X = OAc, Cl)	HCl CH_3-CH(OR)-Cl
Additive	None	(Base) R-COR' (=O) EtO-COEt (=O) ⟨O,O⟩ ⟨O⟩ Et_2O ⟨N⟩ ⟨S⟩ R_2S	(Salt) $R_4N^+X^-$ $R_4P^+X^-$ (X = I, Br, Cl, OAc) --- $R_4N^+ClO_4^-$ $R_4N^+TiCl_5^-$ (without Activator)

Three general methods for living cationic polymerization: classification of initiating systems for vinyl ethers.

Unfortunately, Ivan M Panayotov and Christo B Tsvetanov, the symposium editors, noted that the attendance from the former socialist countries, except Bulgaria, Poland and Hungary, was limited owing to the sever economic situation in these countries.

ISO standards

July 1994 issue

TC45	**Rubber and rubber products**
ISO 3387: 1994	Rubber – Determination of crystallization effects by hardness measurements
TC61	**Plastics**
ISO 4892–2: 1994	Plastics – Methods of exposure to laboratory light sources – Part 2: Xenon-arc sources
ISO 4892–4: 1994	Plastics – Methods of exposure to laboratory light sources – Part 4: Open-flame carbon-arc lamps
ISO 7327: 1994	Plastics – Hardeners and accelerators for epoxide resins – Determination of free acid in acid anhydride

September 1994 issue

TC28	**Petroleum products and lubricants**
ISO 3771:1994	Petroleum products – Determination of base number – Perchloric acid potentiometric titration method
ISO 7536:1994	Petroleum products – Determination of oxidation stability of gasoline – Induction period method
ISO 9200:1993**	Crude petroleum and liquid petroleum products – Volumetric metering of viscous hydrocarbons
ISO 10478: 1994	Petroleum products – Determination of aluminium and silicon in fuel oils – inductively coupled plasma emission and atomic absorption spectroscopy methods
TC 45	**Rubber and rubber products**
ISO 5435: 1994	Rubber compounding ingredients – Carbon black – Determination of tinting strength
ISO 6472: 1994	Rubber compounding ingredients – Abbreviations
TC 61	**Plastics**
ISO 306:1994	Plastics – Thermoplastic materials – Determination of Vicat softening temperature (VST)
ISO 877:1994	Plastics – Methods of exposure to direct weathering, to weathering using glass filtered daylight, and to intensified weathering by daylight using Fresnel mirrors
ISO 4581:1994	Plastics – Styrene/acrylonitrile copolymers – Determination of residual acrylonitrile monomer content – Gas chromatography method
ISO 7765–2:1994	Plastics film and sheeting – Determination of impact resistance by the free-falling dart method – Part 2: Instrumental puncture test
ISO 9772: 1994	Cellular plastics – Determination of horizontal burning characteristics of small specimens subjected to a small flame
ISO 10724:1994	Plastics -Thermosetting moulding materials – Injection moulding of multipurpose test specimens

Electrolyte Data Collection

Dechema has published a two-part volume focusing on a comprehensive collection of properties of electrolyte solutions. Edited by Josef Barthel and Roland Neueder, part 1 includes values of solvent properties and distance parameters, conductivities of dilute and concentrated solutions, transference numbers and limiting ionic conductivities. The data are preceded by a detailed introduction, showing various correlation methods and giving the theoretical basis for the interpretation of the data. Part 2 provides the same data and insight as it relates to ethanol solutions. Both studies conform with the recommendations of IUPAC, and the editors acknowledge the assistance of IUPAC Commission 1.2 Thermodynamics. Pt 1. Conductivities, transference numbers, limiting ionic conductivities, ISBN 3-926959-33-9. Pt 1a Conductivities, transference numbers, limiting ionic conductivities, ISBN 3-926959-39-8. Details available from Dechema, Postfach 150104, D-60061, Frankfurt am Main, Germany.

Declining interest in physical science

The problem of declining public interest in, and awareness of, science is now widely recognized. Indeed, hardly a month goes by without one of the physical or chemical society journals publishing an article bemoaning the declining numbers of young people, particularly the brightest young people, who wish to study the physical sciences at university.

The reasons for this decline and lose of interest in science are complex, however, in many ways they are linked to a lack of communication between scientists and nonscientists and to the strong sense of demoralization found in the scientific community at present. In the developed industrial countries, government spending on research and development has, over the last few years, fallen and is continuing to fall. Due to a lower birth rate, populations are shrinking and tax revenues, which support research and development, are falling. At the same time, due to the success of medical science, people are living longer and healthier lives. Unfortunately, governments have to choose between funding research and funding increasing social security payments and ever increasing pension and health care plans. This is a serious demographic problem which the current high levels of unemployment only serve to exacerbate.

The choice for the government is straight forward, as the people who benefit from these increased social security payments vote, no government would remain popular if it increased taxes to pay for, what most people consider to be unnecessary items such as, research and development. In a democracy, the way out of this dilemma is for the scientists to justify their work and point out to the public (voters) how their work has enriched their lives. On this point, the above mentioned success of modern medicine is something particularly positive. However, such explanations are difficult. Many scientists have problems explaining themselves in words of few syllables to nonspecialists. This inability to communicate is something many have commented upon and is certainly the biggest problem facing publicly funded science.

However, whatever the reasons for this cooling of general interest in science, it is a situation which is unsatisfactory, our society is becoming ever more complex technologically, and there are ever increasing demands for more and more technological advances. Yet even in the technologically advanced societies the general level of scientific and technological literacy is falling. In a world increasingly shaped by science and technology, scientific and technological literacy is a fundamental requirement if people are not to be alienated from the society within which they live, if they are not to be overwhelmed and demoralised by change. This demoralization occurring both by an inability to understand technological advances and also by an inability to come to terms with the moral implications of these advances.

To counter this lack of public appreciation for science and technology, a number of international scientific organizations have, recently, set up working parties to propose solutions; one such is Project 2000+. Project 2000+ is a novel collaboration between a group of major intergovernmental and nongovernmental organizations and agencies with special concerns and responsibilities for science and technology education and research world wide. Its goal is to collaborate at both national and international levels to improve scientific and technological literacy, particularly at the secondary school level.

Paris: a popular venue for meetings of international organizations.

IUPAC is involved in this venture as a member of the International Council of Scientific Unions (ICSU). A meeting was held last summer by all the international agencies involved in Paris, where it was decided that:

1 Ways must be identified for the promotion of scientific and technological literacy for all.
2 Educational programmes, both formal and nonformal, should be put forward which will allow all to satisfy their educational needs and allow them to function effectively in our ever more technologically complex society.
3 To provide guidelines for continuous development of science and technology educators and teachers.
4 To encourage the formation of broadly based national task forces to initiate programmes for greater scientific and technological literacy.
5 To support the development of a wide range of projects designed to promote solidarity and co-operation in achieving scientific and technological literacy for all.
6 Support the evaluation of existing and projected programmes in this vital area.

The 400 participants from the 80 countries who attended the Paris Forum enthusiastically demonstrated their commitment to improving scientific and technological literacy. The Declaration they adopted by consensus at the close of the meeting found its driving force in the World Declaration on Education for All and in the Rio Declaration.

Another such working group has been set up by the International Council of Scientific Unions (ICSU), of which IUPAC is a member. Following the 24th General Assembly of ICSU, a Committee on Capacity Building in Science (CCBS) has been established. This committee contains two Nobel Laureates, L. M. Lederman, Director Emeritus, Fermi Laboratory, USA, and G. Charpak, CERN, France, and several major educationalists from a number of countries.

The CCBS met recently in Paris and identified three clear tasks. The infiltration of science and mathematics in the education of children in primary schools. A major increase in the number and in the richness of linkages to address the isolation of scientists and technicians. To create major instruments for raising the public awareness and understanding of science and technology.

Maison de la Chimie Foundation Prize

The Board of the *Fondation de la Maison de la Chimie* in Paris, France, has decided to award in 1996 the *Grand Prix de la Fondation* which was created in 1985. This prize, worth FRF150 000, is awarded periodically on the initiative of the Board of the Foundation, it is open to one or several candidates, irrespective of nationality, presented by a learned society or a national or international scientific organization. It is one of the most prestigious awards in the field of chemistry, pure or applied, and is awarded for original work in chemistry of benefit to mankind, society or nature.

Entry forms may be obtained from: Fondation de la Maison de la Chimie, 28 rue Saint-Dominique, 75341 Paris Cedex 07, France.

Physical organic chemists drawn to Padua, Italy

One of the world's earliest great physical chemists was an Italian, Professor Joseph Bunnett (University of California, Santa Cruz) reminded delegates in his opening remarks at the 12th IUPAC Conference on Physical Organic Chemistry, held in Padua, Italy, on 28 August – 2 September 1994. Bunnett was referring to Stanislao Cannizzaro of Palermo and Genoa who, in 1858, guided chemists out of an intellectual quagmire relating to atomic and molecular weights. The difficulty, in essence, was the uncertainty as to whether water is HO or H_2O. By reasoning rigorously from Avogadro's hypothesis, Cannizzaro discerned the magnitudes, although not the precise values, of atomic masses and molecular weights as known today. That enabled organic chemists to know how many atoms of each constituent element are present in a molecule. That knowledge was the foundation for theories of bonding and structure from Couper, Kekulé, Butlerow, van't Hoff and Le Bel. Without the clarification that Cannizzaro contributed, organic chemistry as we know it today could not have materialized.

Major contributions to physical organic chemistry have been made by numerous other Italian chemists. The recent Padua conference was informally dedicated to honour two of them who, in a legal sense, are retiring: Professors Giorgio Modena of Padua and Fernando Montanari of Milan. The conference was chaired by Professor Gianfranco Scorrano of Padua, ex-president of the Italian Chemical Society. The participants, about 400, came from 37 nations.

Conference sessions were held in historic buildings in the centre of Padua, with several splendid examples of renaissance art and architecture not far away. The venue for the opening and closing sessions was the University of Padua's magnificent 14th-century Aula Magna in building known affectionately as 'Il Bo' (the ox). Although not the university's first building on its foundation in 1222, it was where Galileo lectured on physics from 1592 to 1610. Eminent former students include Copernicus, William Harvey and Gustavus Aldophus.

Much of modern physical organic chemistry, as developed from the 1920s through to the 1950s, was based on kinetic studies of reactions in solution, also from the kinetic studies of reactions in solution. From the kinetic data, as well as other information, it was often possible to deduce reaction mechanisms. Also, correlation of reactivity data, as dependent upon change of structure, reagent or solvent, enabled quantification of reactivity trends and thereby recognition of subtle features of transition state structure.

Kinetic studies and correlation analysis, in that tradition, were numerous among papers presented in Padua. Some newer paradigms were also represented in force. Theoretical calculations, both by quantum mechanics and molecular mechanics, alone or in connection with experimental evidence, were the substance of many papers. Representative of modern confidence in theoretical calculations is the statement (by Professor Fernando Bernardi of Bologna, and coworkers): 'Several reaction pathways have been fully documented via computation of stationary structures and intrinsic reaction co-ordinates'. In contrast a cynic, with whom many empathized, not so many years ago characterized theoretical calculations as 'the light beyond the tunnel'.

Of other new methods of investigation strongly represented at the conference, prominent were NMR studies, especially to evaluate rate constants and to determine structures of substances in mobile equilibria, besides routine use of NMR to affirm structures of stable molecules. Many studies of mechanism and reactivity of organic compounds with inorganic reagents, in a tradition especially strong in Italy, were reported. Studies of biochemical phenomena by the methods of physical organic chemistry were less strongly represented than one might have anticipated. They have not withered but rather have become so important in biochemistry as often to be reported preferentially at biochemistry conferences.

Other significant contributions came from exploration of organic chemical phenomena by techniques of chemical physics. Those techniques are diverse; among them are studies of ion-molecule reactions in the gas phase by various methods, X-ray crystallography, and a variety of spectroscopic techniques. Professor Curt Wentrup of the University of Queensland, Brisbane, Australia, and co-workers, used yet another: spectroscopic examination of matrix-trapped unstable species. They generated acetylketene by gas phase reactions and co-deposited it with an inert gas on a very cold condenser, so as to form a solid matrix. Examination of the matrix-isolated material revealed the presence of both E and Z conformers.

The 13th IUPAC Conference on Physical Organic Chemistry will be held in Seoul, Republic of Korea, 25–29 August 1996.

French celebrate IUPAC 75th anniversary and Lavoisier bicentenary

More than 500 participants gathered at the Maison de la Chimie, Paris, France, to celebrate both the 75th anniversary of IUPAC and the bicentenary of the execution of Antoine-Laurent de Lavoisier. Claude Fréjacques, vice chairman of the Académie des Sciences and chairman of the Comité National de la Chimie demonstrated how these two historical events are linked together. Lavoisier became the father of modern chemistry with marked contributions from European chemists when chemistry had not yet made its revolution at the end of the 18th century, unlike the other scientific disciplines. He reminded delegates that the Union of Pure and Applied Chemistry was created in 1919 by two industrialists Pope (UK) and Kestner (France), one century later. France has continued to make a major contribution to the Union. Professors Benard and Jeannin have been presidents of IUPAC, and Professors Delaby and Ourisson and M. Gérard have been its General Secretary.

Delegates were told of the main activities of IUPAC both currently as well as its future plans. Professor Guy Ourisson delivered a lecture on the chemical origins of life. He revealed that some of the mysteries associated with the origin of life will be soon explained by chemistry. Professor Hubert Curien, a former Minister of Research, said that chemistry should play a more important role in education. The Lavoisier-IUPAC ceremony, which was also supported by the Minister of Education, was concluded with the unveiling of the Lavoisier statue, sculpted by Zadkine.

Database of kinetic parameters for free radical polymerizations

The IUPAC Macromolecular Division has established a project to collect a critically evaluated database of kinetic parameters for free radical polymerizations. Robert Gilbert, chair of the IUPAC working party on modelling of kinetics and processes of polymerization, under the auspices of Commission IV.2, is inviting all those working in the filed to contribute of information and data to the project. In the first instance, the committee will focus on data for propagation and transfer in homopolymerizations. Those planning to submit information should, in addition to any published work, consider including as completely as possible the specification of their experimental technique, such as monomer purification etc., raw data details, such as GPC traces, information on experimental reproducibility, estimates of uncertainty, and details of the model used to convert data to values of rate parameters.

Professor Gilbert says the committee will use a range of criteria for data evaluation, including whether

or not different techniques are found to yield the same values of rate parameters, and whether data/results submitted give adequate specification of reproducibility and of experimental conditions to enable independent verification and/or recalculation. Those wishing to bring references to the committee's attention, to contribute details of pre-existing and new data, and other supplementary material, or requesting further information, should contact: Professor RG Gilbert, Chemistry School, Sydney University, Sydney, NSW 2006, Australia. Fax +61 2692 3329; E-mail: gilbert_r@summer.chem.su.oz.au.

Role of science in rebuilding countries of FSU probed

Delegates attending a conference on the Role of science in the rebuilding countries of the former Soviet Union, organized by the International Council of Scientific Unions, in co-operation with UNESCO and the DG XII of the European Commission have identified a number of priorities to grapple with the problems facing scientists in the emerging countries. ICSU is very concerned about the problems facing scientists and science in the FSU and is seeking suggestions and comments relating to potential measures that could be taken to alleviate the situation.

At the personal level, delegates believe the brain drain from the FSU can be discouraged by supporting scientists *in situ* or through short term training opportunities abroad. It was also felt that more twinning of professors/chairs from the FSU with institutions in Europe and other countries, and the established and use of e-mail networks should be encouraged. Delegates also agreed that workshops focusing on integration of FSU science into global and international science should be organized, specific seminars, such as one on natural disasters in Asia, should be convened. An independent review of the potential of science in individual countries, and a study of scientific policy structures in the different nations should also be conducted.

Participants also identified what have been described as secondary priorities. These include:

- encouraging investment in the FSU;
- instructing the younger generation on how to function in market economies;
- providing assistance with computerization;
- helping to obtain scientific journals;
- arranging short visits by FSU scientists;
- reusing nuclear weapons testing sites as international research centres on non-military topics;
- providing training in the English language;
- helping spread the word about FSU science and assist in transnational collaboration;
- holding scientific meetings in the FSU;
- providing opportunities for FSU scientists to participate in scientific meetings;
- encouraging participation of FSU scientists in EC research programmes; and
- publishing a directory of institutes and persons in the FSU.

Names and addresses

Full details (names, addresses, telephone/telex/fax numbers, and e-mail) officers of IUPAC bodies were published in *Chem. Intl.* **15**, 215–227 (1993). The IUPAC Secretariat has since been notified of the following changes:

Dr Jo Ann F. Sullivan, Director of Grant Development, Medical University of South Carolina, Charleston, South Carolina, USA. Tel: +1803 7920870. Fax: +1803 7921657. E-mail: Jo Ann sullivan@smtpgw.musc.edu.

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Dr D. S. Moore, Group CST-4, MS-J567, Los Alamos National Laboratory, Los Alamos, NM 87545 USA. Tel: +1505 6671989. Telex: 660495. Fax: +1505 665 4817. Internet: david_moore@cls.lanl.gov.

Prof. W. A. Wakeham, Tel: +44 71 5945556. Fax: +44 71 5945558.

Professor R. Truhaut.

We regret to record the deaths of

Prof. R. Truhaut, France (18 May 1994) – President of Applied Chemistry Division (1963–67)/Member of Division Committee (1957–63) and 1967–69), Committee on SCOPE (1971–75), Coordinating Committee for Analytical Methods for CEE and IARC (1966–77), Section on Food (1961–71), Commission on Food Additives and Contaminants (1957–71), Commission on Toxicology and Industrial Hygiene/Commission on Air Quality (1949–77).

Dr D. A. O'Sullivan, USA (11 September 1994) – Committee on Publications (1981–89).

Commission & Committee News

Organic Chemistry Nomenclature

The Commission on Nomenclature of Organic Chemistry (III.1) met in Balatonfüred (Hungary) on 8th September 1994.

Three documents will be published in *Pure & Applied Chemistry* within the next year.

1 Basic Terminology of Stereochemistry.
2 Glossary of Class Names of Organic Compounds and Reactive Intermediates Based on Structure.
3 Phane Nomenclature, Part 1: Parent Phane Names.

The document, *Nomenclature of Fused and Bridged Fused Ring Systems* is under public review. Two additional documents have recently been finalized by the Commission and will be forwarded for approval by the Division President and IDCNS. These are, *Extension and Revision of the von Baeyer System for Naming Polycyclic Systems and Extension and Revision of the Nomenclature for Spiro Compounds*.

The Commission, jointly with the Commission on Nomenclature of Inorganic Chemistry, is actively engaged in the preparation of a book, *Nomenclature of Organometallic Compounds*. Publication is expected within 3 years.

The Commission has spent some considerable time on the project, *Preferred Names*. A thorough revision of all principles, rules, recommendations and conventions is underway to systematize and simplify the current system. The Commission also examined the Taylor–Godly report on *Fullerene Nomenclature* and agreed on the principles which will lead to a correct nomenclature and pave the way for naming all new structures in this rapidly evolving field of chemistry.

The draft fullerene nomenclature document prepared Taylor and Godly, was discussed in the light of comments received and current *Chemical Abstracts* practice. It was agreed to maintain the relatively narrow definition for fullerenes, and to refer to analogues with ring sizes other than 5 and 6 as quasifullerenes. It was further agreed to keep the naming style in the Taylor/Godly document, without specification of ring size for normal fullerenes. For quasi-fullerenes, ring sizes could be specified in parentheses in front of the parent name. More information was needed about the method of specifying isomers with the same symmetry, by giving the original reference, and possibly by adding an extract from forthcoming *Atlas of Fullerenes*. *Chemical Abstracts* would consider the use of this method when the *Atlas* was available.

It was agreed that both the Taylor and *Chemical Abstracts* numbering methods should be included in the document, without specifying any IUPAC preference. Indeed it seemed that the Taylor approach could be regarded as analogous to 'natural product' numbering as used in Section F, and the *CAS* approach as a more systematic alternative. It was clear that users would wish to derive numberings infrequently, if at all; they would simply use the numbering diagrams provided. Names using *CAS* numbering would be distinguishable by their different use of ring size designators and carbon numbers. Different numbering had been established only for C_{60} and C_{70}; Dr Giles would provide *CAS* numbering for all other systems described in the Taylor/Godly document, and both parties would explore the possibility of an agreement on numbering (e.g. for C_{76}, C_{78} and C_{84}).

Physical Organic Chemistry

The Commission on Physical Organic Chemistry (III.2) met in Padua, Italy, on 2–3 September 1994.

A concern of the commission is the reception given to its reports and recommendations. For example, there is a perception that the proposed *System for Symbolic Representation of Reaction Mechanisms* issued in 1989, is not widely known or accepted in the Chemical community. This system is intended to be more widely applicable and more precise than the traditional system derived by Ingold in the 1930s, and to be used in conjunction with that system, which often has only a loose connection to actual mechanistic details. It was suggested that continuing effort should be made by the Commission to bring such reports to the attention of the Chemical community so that these proposals can be judged on their merits. It was decided that one way to do this would be to contact book authors and publishers, so that they are aware of the recommendations, and could give them broader exposure.

Another action to follow up on a completed project is to begin assembling now a file of comments on the 2nd edition of the *Glossary of Terms used in Physical Organic Chemistry*, issued in 1994, so that any future modifications could be handled in an expeditious manner. Several suggestions have already been received.

Two publications have appeared in *Pure & Applied Chemistry* in 1994, the 2nd edition of the *Glossary of Terms in Physical Organic Chemistry* and a *Compilation and Critical Evaluation of Reactivity Parameters and Equations*. A similar *Compilation of Scales of Medium Effects* is expected to be complete in 1995.

The Commission of Physical Organic Chemistry (III-2). Standing (from left to right) Allende Kim, Baciocchi, Shorter, Ruasse, Perrin, Tee, Siehl, Raber, Kirby and Takeuchi, and sitting (from left to right) Rappoport, Tidwell, Zdysiewiecz and Drenth.

Among the present and future projects of the commission those on Theoretical and Computational Chemistry are of prominent importance. There is a clear need for co-ordination with ongoing projects in the Physical Chemistry Division in these areas.

The commission raised the problem of comparability of levels of education in chemistry in various countries. This problem is of increasing importance because of the greater number of students studying abroad. The problem is a general one applicable not only to organic chemistry, and should be attacked by the IUPAC bureau or the Division.

The 12th International Conference on Physical Organic Chemistry in Padua (28 August – 2 September 1994) was rated as highly successful, reflecting that Physical Organic Chemistry is alive and well. the lectures and communications were well attended by the 374 participants indicating the quality of the programme and its variety of subjects, including ones outside the mainstream of classical physical organic chemistry. It is expected that this widening of scope will continue in future conferences. Two supplementary lectures, one on Hammett and one on Inglod, placed organic chemistry in a historical perspective.

The next meeting will be held in Guildford, UK, 5–7 August 1995, during the IUPAC General Assembly.

Wiendelt Drenth

Data Base of Protein Structures

The IUPAC–IUBMB–IUPAB Interunion Task Group on the Standardization of Data Bases on Protein Structures Determined by NMR in Solution met in Veldhoven, Holland, on 17–19 August 1994.

The agenda of the meeting contained three items, to establish a timetable for the future activities of the Task Group, to finalize the groups Recommendations and to draft a list of addresses for an initial release of these Recommendations prior to publication. It was decided that the finalised Recommendations would be ready for release at the next meeting of the Task Group in Keystone, CO, USA, in early April 1995.

Critically Evaluated Database of Kinetic Parameters for Free-Radical Polymerization

The IUPAC Macromolecular Division has established a project to collect a critically evaluated database of kinetic parameters for free-radical polymerization reactions. An invitation to contribute information and data is issued to all those expert in this field.

Firstly, the committee will concentrate on data for propagation and transfer in homopolymerization. Those wishing to bring references to the committee's attention, to contribute details of pre-existing and new data, and other supplementary material, or just requesting further information about this database, should contact the Project Co-ordinator: Professor R. G. Gilbert, Chemistry School, Sydney University, Sydney, NSW 2006, Australia (fax 61 2 692 3329; E-mail:gilbert_r@summer.chem.su.oz.au).

Those submitting information should, in addition to published references, consider including as completely as possible the specifications of their experimental technique (monomer purification etc.), raw data details (GPC traces), information on experimental reproducibility, estimates of uncertainty, and details of the model used to convert data to values of rate parameters.

A range of criteria will be used by the committee for data evaluation, for example, whether data/results submitted give adequate specification of reproducibility and of experimental conditions to enable independent verification and/or recalculation and whether or not different techniques are found to yield the same values for rate parameters.

Separation Methods in Analytic Chemistry

The inaugural meeting of the Commission on Separation Methods in Analytic Chemistry (v.3) was held in Lund, Sweden, on 25–27 July 1994.

At this meeting the newly constituted Commission on Separation Methods in Analytical Chemistry(V.3) was able to plan ahead with a much greater sense of security than been possible for its predecessor the LLTC in Chromatography and Other Analytical Separations. The uncertainty over the continuation of a commission devoted to analytical separations, which had been present before the General Assembly meeting in Lisbon in 1993, had been resolved. Despite experiencing the hottest day in Lund since records began, the six Commission members who attended the meeting could concentrate on developing a programme for the future.

The Chairman Aurel Marton started the meeting, which was held on the campus of the University of Lund only a short distance from the famous cathedral, by noting that since Lisbon three papers had been published by the Commission in *Pure & Applied Chemistry* on liquid–liquid distribution, SFC/E and analytical pyrolysis. The work of the Commission and in particular the general Nomenclature for Chromatography had also been publicized by the Secretary Roger M. Smith in poster presentations at three major chromatography symposia in the UK and USA. These had attracted considerable interest and in some cases debate. One further project, on definitions for liquid chromatography, stationary phases, had been carried forward from Lisbon. Subsequently three new projects on ion-exchange material by Aurel Marton, non-linear chromatography by Jan Ake Jönsson and analytical chiral separations by Vadim Davankov have been approved as projects. the meeting learnt that work on these topic was developing well.

Much of the meeting was devoted to the discussion of new and future topics but the adoption of a wide programme was hampered by the relatively small membership of the Commission. New projects were put forward on definitions for liquid chromatography mobile phases and size exclusion chromatography. There included:

- Nomenclature for non-linear chromatography (Project 530/5/93);
- Nomenclature/definitions/operational methods of combined chromatography-atomic spectroscopy (Project 530/6/93);
- Liquid chromatography stationary phase classification/characterization Part II. Operational characterization of phases for ion-exchange separations (Project 530/7/93);
- Chiral chromatography (Project 530/8/93).

A number of projects had been proposed in Lisbon as possible future projects and some of these had been developed further:

- classification and characterization of liquid chromatographic mobile phases;
- chelation chromatography.

A number of potential project topics were then considered. However, the amount of work that could be

Photograph of the Commission at Kullen relaxing between official business. L. to R: Davankov, Siskow, Garcia-Domizuez, Smith, Jönsson, and Marton.

undertaken by the Commission was limited by the small active membership and limited number of TMs so that appropriate specialists were not always available:

- capillary electrophoresis and electrochromatography;
- size exclusion chromatography;
- nomenclature of detection in chromatography;
- sample preparation methods for chromatography;
- integrators and quantitative in chromatography;
- updating of chromatography nomenclature;
- field flow fractionation.

The next meeting will be held during the General Assembly at the University of Surrey in Guildford, UK from 5 to 7 August 1995.

Roger M. Smith

Toxicology and the Teaching of Chemistry

The establishment of a glossary of terms used in toxicology as an aid to the teaching of chemistry is a current programme (740/2/93) in the Clinical Chemistry Division (VII).

When the Commission on Teaching (VII) in the Clinical Chemistry Division was wound up in 1989, it was proposed that the teaching interests of the Division should be represented through the Committee on teaching of Chemistry (CTC). Indeed, it was agreed that the teaching interests of all divisions should be covered in this way. Consequently, since 1991 each division has been invited to nominate a representative to CTC. One outcome of this collaboration between the Commissions and CTC was a project agreed at the General Assembly in Lisbon, with the Commission on Toxicology (VII.4) on Toxicology and the Teaching of Chemistry.

In recent years, many countries have passed legislation concerned with safe practice in the working place. In the UK for example, the *Health and Safety at Work Act* was passed in 1974 which required the appointment of safety representatives, the establishment of safety committees and the inspection of the work place by representatives and/ or members of the Safety Committee. This has implications on the handling of chemicals where they are used in the workplace. More recently regulations for the *Control of Substances Hazardous to Health* (COSHH) require laboratories and institutions to compile and retain inventories of chemicals used within their laboratories. This must include statements concerning their toxic properties, safe handling procedures and actions that should be taken in the event of an accident or spillage. The safe handling of potentially toxic biological materials has been dealt with in the UK by the Department of Health and Social Security, which produced a series of documents culminating in *Safe Working and the Prevention of Infection in Clinical Laboratories* which was produced by a Health and Safety Commission. The International Programme on Chemical Safety, which is a Division of the World Health Organization produced international Chemical safety cards in conjunction with the Commission of the European Communities. These are examples of legislation and documentation being produced nationally, in increasing numbers of countries in the world, and internationally through bodies like the World Health Organization.

It is reasonable that chemists should be aware of the dangers of the chemicals that we use within our laboratories, and that there should be documentation and legislation to help this safety conscious process. But this of course is not confined to the laboratory. Chemicals are used increasingly in domestic and non-technical environments, where their safe handling is no longer solely the concern of qualified chemists. For instance, consider the use of domestic cleaners, solvents and detergents, weed killers and pesticides, and proprietary medicines. One may very well ask the question therefore who is the person to whom the public might turn to seek help and advice in the safe handling of chemicals. As like as not the answer that comes back is the chemist. It is not unreasonable that the chemist is seen as the person who can give help and advice on the handling of chemicals, on the toxic effects associated with them, and on how to deal with an incident when it has occurred. On the other hand, this need is not recognized in curricula for the training of chemists, and indeed apart from what they pick up incidentally as part of their educational progress, there is often no formal teaching of toxicology. this can make the chemist particularly vulnerable when his advice is sought. It is difficult to see how there could be a more suited body than IUPAC to address this problem, and a more satisfactory combination than that of CTC and the Commission on Toxicology within the Union, which is why a joint project between the CTC and the Commission on Toxicology was proposed at the 1993 General Assembly.

The proposal states the increasing need for chemists to have a knowledge of toxicology, both for health and safety and for legal reasons. It sets out to address this need in the form of a monograpy to be published on behalf of IUPAC which lays down proposals and guidelines for the inclusion of a syllabus for the basic teaching of toxicology within the tertiary teaching of chemistry.

The monograpy will consists of three main sections as follows:

Curriculum for the teaching of toxicology

A list of topics of which the chemist should have a basic knowledge and understanding. These may be divided

A collection of hazardous domestic chemicals.

into five modules:
- circumstances of poisoning;
- toxic products and their effects;
- toxic pathology and diagnosis;
- environmental toxicology and ecotoxicity;
- toxic hazard and risk assessment.

Chapters on selected topics

This will form the bulk of the monograpy and consists of the following related topics:
- hazards of chemicals;
- toxicokinetics;
- toxicodynamics;
- data interpretation;
- risk assessment;
- risk management;
- exposure and monitoring;
- mutagenicity;
- carcinogenicity;
- reproductive toxicology;
- immunotoxicology;
- skin toxicology;
- respiratory toxicology;
- hepatotoxicity;
- neurotoxicity;
- behavioural toxicity;
- ecotoxicity;
- radionuclides;
- biocides;
- safe handling of chemicals.

Glossary of terms used in toxicology

This will be an abridged version of *Glossary of Terms Used in Toxicology* which has already been prepared and published by the Commission on Toxicology.

The second section will be multi-author with the Commission inviting contributors who are well recognized for their expertise in their particular field. The Commission will also be responsible for outlining a first draft, which will be circulated to members of CTC for comment making use of their teaching background and expertise.

It is hoped that this will be a prime example of the Union using the combined skills of one of its standing committees and commissions in producing a publication to the benefit of the teaching of chemistry internationally, and at the same time addressing the problem of the changing requirements of chemistry within society.

J. H. Duffus
H. G. J. Worth

Food Chemistry

The Food Chemistry Commission (VI.I) of the Applied Chemistry Division met in Norwich, UK, on 2–4 September 1994 to consider future plans.

The programme of the Commission on Food Chemistry was reviewed in depth during its meeting at the CSL. Food Science Laboratory of the UK Ministry of Agriculture Fisheries & Food. Detailed reports and discussion on each of the completed and current projects and consideration of proposals being developed for new projects took place in the context of progressively wider questions about:

1 the present focus of the Commission's work on methods for food analysis;

2 the need to enlarge the Commission's work on methods for food analysis so as to cover new areas;

3 extending it's work to cover new areas in the development of harmonized protocols (e.g. for confirmation of analyte identity and procedures for 'correction for recovery' of analytical measurements, criteria for standard/reference materials);

4 extension of the programme into non-analytical aspects of food chemistry, e.g. speciation and the chemistry of food component bioavailability in the diet;

5 the need to reverse the present fragmentation between Commissions and Divisions of work relating to food chemistry;

6 consideration of the pressures for re-structuring within IUPAC and their implications for food technology;

7 the orientation of IUPAC's work on food chemistry in response to strategies emerging from decision at the UN Conference on the Environment and Development (Rio de Janeiro 1992).

The Commission is developing plans for the 9th International Symposium on Mycotoxins and Phycotoxins to be held in Rome on 28 May – 2 June 1996 in association with and FAO Workshop on analytical methods for these contaminants.

Detailed planning is in progress for UNESCO-funded training programmes on food monitoring pro-

grammes for ochratoxin and for cigutera toxins. Preliminary plans are being developed for a Workshop for experts from developing countries aimed at identifying their needs for food analyses: emphasis will be on identifying needs for capacity-building for locally sustainable food monitoring programmes.

Environment-related problems will not be forgotten – proposals are being developed for a major project on the implications of recycling of packaging for the food industry, food safety and the consumer.

The next meeting will be in Guildford, UK on 5–7 August 1995.

David McWeeny

Equilibrium Data

The Commission on Equilibrium Data (V.6) of the Analytical Chemistry Division met in London, UK, on 27–28 August 1994.

The Stability Constants Database, SC-database (IUPAC/Academic Software, 1993) is seen as focal point and catalyst for many future initiatives by V.6. SC-database covers the literature for metal (and H^+) – ligand equilibria for the years 1974–89. Data for later years are being added, and inclusion for the 4 earlier book volumes (1895–1973) is well advanced (they will be included in the second release, autumn 1995).

The distinctive contribution which V.6 can make to the Analytical Division is a pool of expertise on equilibrium speciation; SC-database will be an important factor underpinning future horizontal links with other Commissions. V.6 identified horizontal links an important base for future project development.

The Commission should to identify potential users of SC-database so that the product could be tailored to their needs. A number of modifications were initiated, including (I) an expanded package to interpret multicomponent metal/ligand systems and provide pM values for environmental and physiological systems (ii) designation of additional ligand classes, and (iii) an upgrade of the manual with additional tutorials and additional appendices providing advice to users on matters such as the effect of ionic strength, solvent dielectric and temperature on log K values. A working group is to establish criteria for 'evaluation' of data in SC-database so that it can provide the user with 'recommended' values.

The Commission resolved that the past strategy for *Critical Evaluations of Stability Constants* is too slow and the output too small. It discusses whether the publication of long evaluations for tightly focused systems is still relevant. As well as accelerating the compilation phase of an evaluation it was recognized that SC-database may provide a regularly updated vehicle for 'publishing' these evaluations.

A proposal for a new project on 'Influence of pressure on chemical equilibria in aqueous solutions, with particular reference to sea water' was approved by the Commission. Preparation of discussion papers on possible new projects on 'Surface complexation' and 'Host–guest interactions' was initiated.

The next meeting will be held in Guildford on 5–7 August 1995

Kip Powell

Erratum

There is an incorrect title on page 138 of the *IUPAC Handbook 1994–1995*, whereby the Current Programmes for the Commission on Macromolecular Nomenclature (IV.1) has the incorrect heading 'Working Party on Structure and Properties of Commercial Polymers'. The latter heading is repeated correctly on page 139. Our apologies for the confusion.

Organosilicon Chemistry Poznan, Poland 15–20 August 1993

The 10th International Symposium on Organosilicon Chemistry was held at the Adam Mickiewicz University, Poznan, Poland.

It was organized by the Adam Mickiewicz University. Chairman of the Symposium was Professor Bogdan Marciniec. The Symposium was held under the auspices of IUPAC. The IUPAC representative was Professor Edward Grazywa. Chairman of the National Scientific Committee was Professor Zygmunt Lasocki. The International Advisory Board of the Symposium was composed of about 40 outstanding specialists in the field of the organosilicon chemistry from 15 countries of Europe, America and Asia.

The Symposium was the 10th jubilee world gathering of scientists having interest in the broad area of organosilicon chemistry. The organization of scientific meetings of the series at regular 3 years intervals since the first Symposium organized in Prague (then Czechoslovakia) in 1965, has now become a firm tradition. These subsequent symposia were organized in various countries of Europe, in United States and in Japan. The last one was held in Edinburgh (UK) in 1990, while the place for the next one planned for 1996 is Montpellier (France).

The Poznan Meeting attracted a broad variety of participants, about 500 from 27 countries, representing both academic and industrial research centres. The scientific programme included 4 plenary lectures and 34 invited lectures, 80 oral presentations about 180 posters. the Symposium pulled together current re-

search in various areas of silicon chemistry, such as synthesis properties and reactions of organosilicon compounds, use of silicon reagents in organic synthesis, silicon biochemistry, theoretical aspects of the structure and reactivity of silicon compounds including reactive intermediates, silicon based polymers and their application in material science and the technology and variety of applications of silicon based materials – known under the names of silicone. The creation of an opportunity for scientists of diverse backgrounds and various interests related to silicon chemistry was the primary goal of the Symposium. The date of the Poznan Symposium coincided with 50th Anniversary of the discovery of 'direct synthesis' of silicone monomers, which had a great impact upon the development of the organosilicon chemistry. On this occasion the Symposium programme included a special session devoted to the history of organosilicon chemistry which was attended by Eugene Rochow (USA) and Richard Muller who were independently responsible for this important invention. Professor Rochow gave recollections of his earlier career and who drove him to the discovery of the 'direct synthesis'. Other prominent organosilicon chemists: Mikhail Voronkov (Russia), Gerard Fritz (Germany), Robert West (USA), Cecil Frey (USA) and Bernard Kanner (USA) were presenters in this session.

Plenary and invited lectures to this Symposium represented various scientific and technological aspects of the chemistry of silicon. They were delivered by outstanding specialists in this broad and rapidly progressing field.

A considerable part of these presentations was devoted to synthetic problems of the modern organosilicon chemistry. Nils Wiberg (Germany), the last Kipping Prize winner, in the first plenary lecture introduced the audience to the intriguing chemistry of sterically crowded supersily compounds. His presentation was followed by contributions covering some other challenging problems of synthesis and reactions of organosilicon chemistry, such a new synthetic possibilities using metal catalysts (lectures by: Jacques Dubac, France; Mitsuo Ishikava, Japan; Ulrich Schubert, Germany; T. Don Tilled, USA), pentacoordinate silicon chemistry (Reinhold Tacke, Germany; Vadim Pestunovitch, Russia), stereochemistry of silicon compounds (Ian Fleming, UK; Heideki Sakurai, Japan), unusual transformations of silicon compounds (Tom Barton, USA; Michael Lappert, UK; Robert West, USA), heteroatom silicon chemistry (Hubert Schmidbaur, Germany); silylene reactions (Shi Ando, Japan), silyloanion chemistry (Kohei Tamao, Japan) and some biological aspects (Edmund Lukevich, Latvia).

A substantial number of the presentations were related to physical organosilicon chemistry, Alan Bassindale (UK) in his plenary lecture reviewed dynamic NMR studios of solvation to basic problems of mechanistic pathways of the substitution at the silicon centre. Mechanistic problems of silylene reactions were tackled by Peter Gaspar (USA) and those of hydrosilylation reactions were discussed by Kenrick Lewis (USA). Structural studies of organosilicon compounds were the subject of Hans Bock's (Germany) and Wieslaw Wojnowski's (Poland) presentations while structural effects on reactivity and spectral properties were treated by Klaus Buhlmann (Germany) and Jano Schraml (Czech Republic). Theoretical organosilicon chemistry was represented by Yitzaak Apeloig (Israel), who gave accounts of his recent studies on the reactivity of unstable silicon intermediates.

The progress in organosilicon chemistry is directly related to its practical aspects. Search for new silicon-based polymers and new useful silicon materials for a variety of applications have been the driving force for fundamental research in silicon chemistry. Recent achievements in industrial silicon polymer science were reviewed in the plenary lecture delivered by James White (UK) from Dow Corning Company, the leading manufacturer of silicones. The fundamental research on silicon polymers was the subject of several presentations. Three of them were devoted to synthesis of oligo and polysilanes (lectures of Joyce Corey, USA; Krzysztof Matyjaszewski, USA; and Edwin Hengge, Austria). Olefin metathesis route to polycarbosilanes was reviewed by Filkensthein (Russia). Synthesis of precursors for ceramic materials and their transformation by pyrolytic processes were subjects of presentations of Robert Corriu (France) and Jean Paul Pillot (France). The lecture on synthesis of new polysiloxanes and polymetallosiloxanes was delivered by Alexander Zhdanov (Russia). There is currently great interest in chemical vapour deposition processes using organosilicon compounds. This topic was represented in Hideomi Koinuma's (Japan) talk. The research closely related to the technology and applications of silicon based material – silicones, was the subject of lectures of representatives of important industrial research centres: Masayuki Ikeno Shin-Etsu (Japan); Hans Mayer, Wacker (Germany), Jean Marc Pujol, Rhone Poulenc (France); Gunnar Schuesler, Elkem (Norway).

The growth of organosilicon research throughout the world has been remarkable in recent years. The Xth Organosilicon Symposium on Organosilicon Chemistry summarized the recent progress in this field and provided insight into the possible direction for its future scientific and technological development. A special session was devoted to perspectives in organosilicon chemistry. The discussion was moderated by Tom Barton (USA). Several outstanding specialists from academic and industrial research centres presented their views on these perspectives.

38th IUPAC General Assembly, Guildford '95

IUPAC General Assemblies are held in odd-numbered years. The next such assembly, the 38th General Assembly, will take place in Guildford, UK, during August 1995.

The General Assemblies of IUPAC consist of a set of meetings of the Union's Council, Bureau and Committees. At any one moment during the General Assembly, there may well be over 30 meetings taking place simultaneously. Only members of IUPAC bodies, such as Commissions and Committees, together with National Representatives and invited observers may attend these meetings.

The last General Assembly, the 37th, was held in Lisbon, Portugal, hosted by the *Sociedade Portuguesa de Quimica* and the Department of Chemistry of the Faculty of Sciences of the University of Lisbon. The 38th General Assembly is being hosted by the University of Surrey, Guildford, and organized by the Royal Society of Chemistry in collaboration with the Department of Chemistry, and the Conference Office of the University of Surrey.

The University of Surrey is a modern facility which occupies a commanding position on hills outside the town of Guildford, in the county of Surrey, which is an attractive historic town some 30 miles south west of London. The country side around Guildford, the rolling South Downs and Weald, is well known for the fine quality of its country houses and gardens.

Access to the town and university are excellent. There are good road and rail links with central London. Guildford being less than 45 minutes by rail from Waterloo station on the south bank of the Thames, and within an hour's travelling time of Heathrow and Gatwick airports, both of which are served by regular and rapid coach and rail links. There is an hourly train service from Gatwick airport to Guildford. From Heathrow, one would take a bus to Woking railway station (30-minute bus service, Railair, which runs from 09.30 to 18.30), and then a train to Guildford.

Once in Guildford, there is a special Link bus service, yellow and green minibuses run at regular intervals between the university, the rail and bus stations and the town centre.

Details

Well before the General Assembly, participants with any questions concerning reservation of accommodation, meals, etc., should contact the Royal Society of

Guildford: site of the 38th IUPAC General Assembly.

Chemistry (see address below). From 31 July 1995 all queries should be addressed to, The Registration Desk in the social area of the Continuing Education Centre which is situated on the second floor of the Senate House of the University of Surrey. Any questions concerning the Schedule of Meetings, the locations of meeting rooms or IUPAC business should be addressed to the IUPAC Secretariat in Oxford until 28 July 1995, and from that date to the IUPAC Secretariat situated in the social area of the Continuing Education Centre.

The Participation Questionnaire should be completed and returned, to reach the Oxford Secretariat by 31 December 1994 or as soon as possible thereafter, even for those unable to attend the General Assembly.

Only members of IUPAC bodies and invited observers, together with their accompanying persons may attend the General Assembly. Requests to reserve student accommodation should be made as soon as possible indicating preferences. Similarly, persons desiring special diets can only have these provided if advance notice is given to the organizers. The completed Reservation form, together with the appropriate deposit (for student accommodation this deposit is GBP50 per person) should be returned, by 31 December 1994, to:

Dr John F. Gibson
Secretary (Scientific)
The Royal Society of Chemistry
Burlington House
London W1V 0BN, UK
Tel: (44) 171 4378656
Fax: (44) 171 7341227

All university accommodation facilities are only a few minutes walk from the restaurant and meeting place locations. The student accommodation is basic, there are only a few rooms with *en suite* facilities, and are generally of single occupancy. There are a limited number of duplex or double rooms, however, these will be allocated on a first come, first served basis. All keys will be supplied at registration at the Continuing Education Centre.

All cheques and money orders should be made payable to The Royal Society of Chemistry. Participants transferring money from overseas are reminded that bank charges are levied. These charges are usually deducted by the bank before passing on the money to the Society.

Participants are requested to ensure that any cheques or money orders sent independently of their application forms be marked with the Applicants name and with 38th IUPAC General Assembly.

We recommend that applications be made for a visa no later than three months before the General Assembly, and if a visa has not been granted by 1 month prior to departure, the IUPAC Secretariat should be notified by the applicant.

For Titular Members who have requested travel and/or subsistence aid to be paid in cash in pounds sterling, the cheques will be distributed by Mrs. Erica Sheppard in the IUPAC Secretariat. These cheques may be cashed at the University branch of the National Westminster Bank.

If cancellations are received at the Royal Society of Chemistry after Thursday 29 June 1995 a refund cannot be guaranteed.

Invitation to Affiliates to attend the General Assembly

On the occasion of the 38th IUPAC General Assembly, Affiliates are invited to participate, as observers, in the meeting of the IUPAC bodies in whose work they are interested. The names and addresses of the Chairpersons of IUPAC bodies were published in *Chem. Int.* **15**, 216–227 (1993) and subsequent issues will contain details of any changes of address.

Advance approval of the Chairperson of the relevant body should be sought and obtained before an observer may attend a meeting; a copy of the letter should be sent to the IUPAC Secretariat. Copies of Chairpersons' replies should also be sent to the IUPAC Secretariat, and if permission is granted the Affiliate observer will be sent the Information Booklet, Accommodation Reservation Form, etc., so that attendance may be confirmed to the IUPAC Secretariat.

Services Operating During the General Assembly:

Mailing Address
38th IUPAC General Assembly
c/o Conference Office
University of Guildford
Guildford
Surrey GU2 5XH, UK

Telephone
IUPAC Secretariat (44) 1483 259338
Registration/Information desk (44) 1483 259337
FAX (44) 1483 579266

A flat rate, per page, for messages faxed will be charged. All faxes must be paid for in advance.

4th International Conference on Heteroatom Chemistry (ICHAC-4) Seoul, Korea 30 July– 4 August 1995

This IUPAC sponsored conference will be held in collaboration with the Korean Chemical Society, Korean Pharmaceutical Society, the Centre for Biofunctional Molecules and the Organic Chemistry Research Centre.

The conference covers chemistry and biochemistry of heteroatom compounds including nitrogen, sulphur, silicon, selenium, boron, halogens, alkali metal and other elements. Emphasis is given to:

- synthesis;
- reactions;
- structures;
- reaction mechanisms;
- physical properties;
- biologically active compounds;
- biofunctional molecules;
- new materials applications to pharmaceutical, agricultural, and other industrial purposes.

The conference will be held at the Sheraton Walker Hill Hotel in Seoul, the ancient capitol city dating back to the 14th century and various events are planned to coincide with the 600th anniversary of the founding of the capitol city. Seoul is rich in vibrant Korean tradition of artistic and musical culture, that blends with modern culture and technology. the important sight seeing places include the Royal Palace with its gardens, the National Museum, the Olympic park and many other historic places.

All persons wishing to participate in the conference are kindly requested to contact: professor Kyongtae Kim, Secretary general, ICHAC-4, Department of Chemistry, Seoul National University, Seoul 151–742, Korea (Tel: 82 2 880 6636 Fax: 82 2 874 8858).

Colloquium Spectroscopicum International XXIX Leipzig, Germany 27 August– 1 September 1995

This IUPAC sponsored conference is being run in collaboration with the, Deutscher Arbeitskreis für Angewandte Spektroskopie in the Fachgruppe Analytische Chemie of the Gesellschaft Deutscher Chemiker, the University of Leipzig, the ISAS, Dortmund and Berlin, together with the UFZ, Leipzig-Halle.

The congress aims to encompass all areas and all aspects of analytical spectroscopy, from fundamentals and instrumentation to applications in the vast variety of primarily elemental analysis. Amongst these are biology, medicine and environmental studies, together with geology and metallurgy. As with the previous meetings in this series, the CSI XXIX will bring together specialists from all over the world, who develop techniques or who apply these techniques to solve particular problems, from universities, other research institutes and from industry. The scientific programme comprises plenary and other invited lectures, contributed posters, discussions and an exhibition of analytic spectroscopic equipment. Four Post Symposia, to be held in different places, will provide a more detailed view on some specific techniques.

Any one topic will be considered in depth, that is, current advances in methods, techniques, sampling, data handling and theories. Some of the topics to be considered include:

- atomic emission and fluorescence, plasmas and discharges;
- laser spectroscopy;
- X-ray, gamma, photoelectron and auger-electron spectroscopy;
- diffraction techniques;
- elemental mass-spectroscopy;
- molecular spectroscopy.

Also, progress in solving analytical problems in the following fields will be considered:

- trace analysis;
- local and micro analysis;
- distribution and surface analysis;
- speciation;
- chemometrics, modelling.

An exhibition of analytical spectroscopic instruments, accessories, software, literature and various other items is planned. There are four post symposia, they are:

- Electrothermal Atomization in Analytical Atomic Spectroscopy (Würzburg, 3–5 September 1995);
- Laser Techniques in Analytical Atomic Spectroscopy (Berlin, 1–3 September 1995);
- Analytical Applications of Glow Discharges in Optical and Mass Spectroscopy (Dresden, 1–4 September 1995);
- ICP-MS (Weringerode/Harz, 1–4 September 1995).

Leipzig is one of the great cities of eastern Germany,

Statue of Gottfried Wilhelm Leibniz (1646–1716) in front of Leipzig University's main building.

it had been granted a market as early as 1165, which soon developed into the famous trade-fair. Over the centuries Leipzig has accumulated a rich cultural heritage. The university, the venue for this conference, was founded in 1406; and amongst its old students it numbers Agricola, Leibnitz, Ostwald and Hertz. Auerbach's Keller, notorious from the legend of Dr Faust, was an important meeting place for students and writers. However, probably the most famous resident of Leipzig was Johann Sebastian Bach, organist of St. Thomas' Church and master of the Thomaner-Chor. Concerts of this renowned choir and of the celebrated Gewandhaus-Orchester are among the traditional highlights of a visit to Leipzig.

For further information please contact: President, CSI XXIX, Professor H. Nickel, IWE-KFA, D-52425 Jülich, Germany (Tel: +49 2461 61 5565 Fax: +49 2461 61 3699 E-mail (Internet): h.nickel@kfa-juelich.de (bitnet): rws086@djukfa11.bitnet) and CSI XXIX Secretariat, GDCh, Abt. Tagungen, Postfach 90 04 40, D-60444 Frankfurt/M, Germany (Tel: +49 69 7917 358 Fax: +49 69 7917 475 Telex: 4170 497 gdch d).

Industry–Education Initiatives in Chemistry Partners in Chemical Education
York, UK
29 August– 2 September 1995

This is the first international conference sponsored by IUPAC which specifically aims to promote links and dialogue between concerned industrialists and teachers from higher education, secondary and primary schools, and educational decision makers; and to evaluate and encourage good practice and discuss issues of collaboration between industry and education.

The organisers are the IUPAC Committee on the teaching of chemistry, The Royal Society of Chemistry and the University of York. This conference will consist of plenary lectures, symposia, work shops and poster sessions. In addition, there will be a number of visits to industrial sites, lectures on frontier areas of industrial chemistry and both formal and informal group meetings.

The conference will focus on:

- Education about industry, learning what industry does and how it does it, learning about the processes, the important legislation and future targets. Helping to up-date teachers and educators about current industrial practice.
- Education through industry, using industrial practice, stories and activities to bring alive chemistry, and science in general, curricula.
- Education for industry, exploring teaching strategies which can help students develop skills needed in industry.
- Education within industry, examination of the education and training provided within industry for its employees.
- Education for industrialists, looking at what is currently happening within chemistry curricula and who it will effect future employees.

A number of workshops have already been organized (up to twenty can be accommodated), these include:

- Project 2000+: Education and industrial aspects of chemistry (UNESCO and ICASE);
- Industrial Case Studies for Undergraduate Courses [Reiko Isuyama (Brazil) and Gordon Fettes (UK)];
- The Zeneca Project: Use of Chemicals in Agriculture [Graham Wilson and Jack Holbrook (ICASE)];
- Total Quality Management – an effective tool for schools and industry [Chemical Manufactures' Association (US)];
- Engineers have a constructive role in supporting what is taught in primary schools (British Petroleum).

The registration fee will be about USD340 (or USD260 for IUPAC Affiliates and RSC Members) for full participation and USD75 for accompanying persons. Accommodation and meals on the campus of the University of York for the period of the conference will be about USD300. There will be a limited number of grants for school teachers and for participants from developing countries.

The city of York was founded by the Romans who called it Eboracum. It lies 200 miles north of London, half way to Edinburgh. Its Roman heritage, it was the site where the young Constantine was declared Emperor of the Roman world, is now overshadowed by the significant recent discoveries of the Viking or Norse civilization of this town. The city is dominated by York Minster, one of the largest and finest Gothic cathedrals, and by the ancient city wall, much of which may still be walked.

Near York lie the Yorkshire Moors and dales, well known to those who have read the novels of James Herriott. Nearby, is Whitby, a small, beautiful harbour town near where Captain James Cook was born; Castle Howard, a magnificent county house celebrated in the television adaptation of Waugh's *Brideshead Revisited*; Howarth, the home of the Brontes; and the lovely and haunting ruined abbeys of Riveaulx and Fountains.

For more information please contact: Dr J. F. Gibson (Conference Arrangements), The Royal Society of Chemistry, Burlington House, Piccadilly, London WIV 0BN, UK (Tel: +44 71 437 8656 Fax: +44 71 734 1227) or Professor D. J. Waddington (Academic Matters), Department of Chemistry, University of York, Heslington, York YO1 5DD, UK (Tel: +44 904 432 600 Fax: +44 904 432 605).

Conference Calendar

1995

Macrocyclic chemistry
2–7 July
20th International Symposium on Macrocyclic Chemistry. Jerusalem, Israel.
Prof. D. Meyerstein, Chemistry Department, Ben-Gurion University of the Negev, PO Box 653, Beer-Sheva 84105, Israel. Tel: +972 (7) 461238 Fax: +972 (7) 237682

Polymer morphology and electrical properties

5–7 July
International Symposium on Polymer Morphology and Electrical Properties. Lodz, Poland.
Prof. A. Galeski, Centre of Molecular & Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, 90–363 Lodz, Poland. Tel: +48 (42) 818952 or 815761. Fax: +48 (42) 847126 or 815483. E-mail: julanski@lodzl.p.lodz.pl.

Analytical chemistry

9–15 July
SAC 95: International Conference on Analytical Chemistry. Hull, UK.
Prof. A. Townshend, School of Chemistry, University of Hull, Hull HU6 7RX, UK. Tel: +44 (482) 465027. Fax: +44 (482) 466410.

Toxicology and clinical chemistry of metals

10–13 July
5th COMTOX Symposium on Toxicology and Clinical Chemistry of Metals. Vancouver, BC, Canada.
Prof. F. W. Sunderman, Jr., Departments of Laboratory Medicine and Pharmacology, University of Connecticut Medical School, Post Office Box 1292, Farmington, Connecticut 06034–1292, USA. Tel: +1 (203) 792328. Fax: +1 (203) 6792154.

High swelling gels

10–14 July
36th Microsymposium on Macromolecules – High Swelling Gels. Prague, Czech Republic.
Prof. B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague 6-Petriny, Czech Republic. Tel: +42 (2) 360317. Fax: +42 (2) 367981.

Functional dyes

16–21 July
3rd International Symposium on Functional Dyes (Functional Dye '95). Santa Cruz, California, USA.
Dr J. Pacansky, IBM – Almaden Research Centre, K42/803, 650 Harry Road, San Jose, CA 95120–6099, USA.

Heteroatom chemistry

30 July – 4 August
4th International Conference on Heteroatom Chemistry. Seoul, Korea.
Prof. Kyongtae Kim, Secretary General, ICHAC-4, Department of Chemistry, Seoul National University, Seoul 151–742, Korea. Tel: +82 (2) 880 6636. Fax: +82 (2) 874–8858.

Novel Aromatic Compounds

31 July – 4 August
8th International Symposium on Novel Aromatic Compounds (ISNA-8). Braunschweig, Germany.
Prof. H. Hopf, Institut für Organizche Chemie, Technische Universität, Hagenring 30, D-38106 Braunschweig, Germany. Tel: +49 (531) 391 5255. Fax: +49 (531) 391 5388

IUPAC General Assembly

4–11 August
38th IUPAC General Assembly. Guildford, Surrey, UK.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion

Organometallic chemistry directed toward organic synthesis

6–10 August
8th IUPAC Symposium on Organometallic Chemistry directed toward Organic Synthesis (OMCOS-8). Santa Barbara, California, USA.
Prof. B. H. Lipshutz, Department of Chemistry, University of California, Santa Barbara, California 93106–9510, USA. Tel: +1 (805) 8933072. Fax: +1 (805) 8937287. E-mail hr03conf@ucsbvm.ucsb.edu.

Heterocyclic chemistry

6–11 August
15th International Congress of Heterocyclic Chemistry. Taipei, Taiwan, China.
Prof. Chin-Kang Sha, Department of Chemistry, National Tsing Hua University, Hsinchu 300, Taiwan, China. Tel: +86 (35) 722427. Fax: +86 (35) 725870. E-mail: cksha@chem.nthu.edu.tw.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy.

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

35th IUPAC Congress

14–19 August
35th IUPAC Congress. Istanbul, Turkey.
Prof. Yüksel Inel, Chemistry Department, Bogaziç University, P.K.2 Bebek 80815, Istanbul, Turkey. Tel: +90 (1) 2631500 or 2631540, ext. 1619 (direct) or ext. 1610 (secretary). Fax: +90 (1) 2659778 or 2656357. E-mail: INEL@TRBOUN

Plasma chemistry

21–25 August
12th International Symposium on Plasma Chemistry. Minnesota, Minneapolis, USA.
ISPC-12, c/o Catherine Ploetz, 218 Nolte Centre, University of Minnesota, 315 Pillsbury Drive SE, Minneapolis, MN 55455, USA.
Tel: +1 (612) 626 2259. Fax: +1 (612) 626 1632.
Internet: ispc12@pdcs.cee.umn.edu

Spectroscopy

27 August – 1 September
29th Colloquium Spectroscopicum Internationale. Leipzig, Germany.
Prof. H. Nickel, Forschungszentrum Jülich GmbH, Institut für Werkstoffe der Energietechnik, RWTH Aachen, D-52425 Jülich, Germany.
Tel: +49 (2461) 615565. Fax: +49 (2461) 613699.

Liquid and Amorphous Metals

27 August – 1 September
9th International Conference on Liquid and Amorphous Metals. Chicago, USA.
Drs Saboungi and Price, Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA.
Tel: +1 (708) 252 4341 (M.-L. Saboungi), +1 (708) 252 5475 (D. L. Price)
Fax: +1 (708) 252 7777 (both)

Industry – education initiatives in chemistry

28 August – 2 September
International Symposium on Industry – Education Initiatives in Chemistry. York, UK.
Dr J. F. Gibson, The Royal Society of Chemistry, Burlington House, Piccadilly, London WIV OBN, UK.
Tel: +44 (0)71 4378656.
Fax +44 (0)71 7341227.

Solution Chemistry

29 August – 3 September
24th International Conference on Solution Chemistry. Lisbon, Portugal.
Prof. César A. N. Viana, CECUL – Faculdade de Ciencias, Universidade de Lisboa, R. Escola Politécnica, 58, 1294 Lisboa Codex, Portugal.
Tel: +351 (1) 608823. Fax: +351 (1) 7977837

Medicinal chemistry

3–8 September
AFMC International Medicinal Chemistry Symposium (AIMECS 95). Tokyo, Japan.
Prof. S. Ikegami, Secretary General, AIMECS 95, c/o Faculty of Pharmaceutical Sciences, Teikyo University, Sagamiko, Kanagawa 199–01, Japan. Tel: +81 (426) 850161. Fax: +81 (426) 851870.

Ionic polymerization

4–8 September
1st International Symposium on Ionic Polymerization. Istanbul, Turkey.
IUPAC International Symposium on Ionic Polymerization, c/o Prof. Y. Yagci, Istanbul Technical University, Faculty of Science, Department of Chemistry, Maslak 80626, Istanbul, Turkey.
Tel: +90 (212) 285 32 41. Fax: +90 (212) 285 63 86.
E-mail: Feyusuf@TRITU

Applications of the Mössbauer effect

10–16 September
International Conference on the Applications of the Mössbauer Effect (ICAME-95). Rimini, Italy.
Prof. I. Ortalli, University of Parma, Istituto di Scienze Fisiche, Via M. D'Azeglio, 85, 43100 Parma, Italy.

Bioorganic chemistry

17–23 September
3rd International Symposium on Bioorganic Chemistry. Dagomys, Sochi region of Black Sea Coast, Russia.
Prof. V. T. Ivanov, Shemyakin & Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Ul. Miklukho-Maklaya, 16/10, 117871 Moscow V-437, Russia.
Tel: +7 (095) 335–1511, 330–6338, 330–2800. Fax: +7 (095) 310–7007

Chromatography of polymers

18–22 September.
International Symposium on Chromatography of Polymers and Related Substances. Bratislava, Slovakia.
Dr D. Berek, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, Sk-842 36 Bratislava, Slovakia. Tel: +42 (7) 3782306. Fax: +42 (7) 375923.

Environmental Catalysis

25–27 October
2nd International Forum on Environmental Catalysis. Tokyo, Japan.
Prof. Makoto Misono, Department of Applied Chemistry, Faculty of Engineering, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan. Tel: +81 (3) 3812 2111 Ext. 7272. Fax: +81 (3) 5802 2949.

Automation and New Technology in Clinical Laboratory

2–4 November 1995
6th International Congress on Automation and New Technology in Clinical Laboratory. Sitges, Barcelona, Spain.
Dr F. Javier Gella, BioSystems, S.A., Costa Brava 30, 08030 Barcelona, Spain. Tel: +34 (3) 3110811. Fax: +34 (3) 3117609.

1996

Free-radical polymerization

26–31 May
2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism. Santa Margherita Ligure, Genoa, Italy.
Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy.
Tel: +39 (79) 229556. Fax: +39 (79) 229559

Organic synthesis

30 June – 4 July
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Prof. W. N. Speckamp, University of Amsterdam, Laboratory of Organic Chemistry, Nieuwe Achtergracht 129, 1018 WS Amsterdam, Netherlands.
Tel: +31 (20) 525 5479. Fax +31 (20) 525 5670

Catalysis

30 June – 5 July
11th International Congress on Catalysis.
Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520–8286, USA.
Tel: +1 (203) 432 4378. Fax: +1 (203) 432 4387.

Sweeteners

14–20 July
International Symposium on Sweeteners. Jerusalem, Israel.
Prof. R. Ikan, Department of Organic Chemistry, Hebrew University, Jerusalem 91904, Israel.

(Bio)degradable polymers

15–18 July
37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects.
Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic.

Macromolecules

4–9 August.
36th International Symposium on Macromolecules. Seoul, Republic of Korea.
Dr Kwang Ung Kim, Secretariat of IUPACMACRO SEOUL'96, Division of Polymers, Korea Institute of Science & Technology, P. O. Box 131 Cheongryang, Seoul 130–650, Korea. Tel: +82 (2) 957 6104.
Fax: +82 (2) 957 6105. E-mail: iupac@kistmail.kist.re.kr

Coordination chemistry

18–23 August
31st International Conference on Coordination Chemistry. Vancouver, Canada.
31st ICCC Secretariat, UBC Conference Centre, 5961 Student Union Boulevard, Vancouver, BC, Canada V6T 2C9.
Tel: +1 (604) 822 1050. Fax: +1 (604) 822 1069

Physical organic chemistry

25–29 August
13th International Conference on Physical Organic Chemistry. Seoul, Republic of Korea.
Prof. J. Suh, Department of Chemistry, Seoul National University, Seoul 151–742, Republic of Korea. Tel: +82 (2) 8806642. Fax: +82 (2) 8891568.

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* **14**, 203 (1992).

International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

President: K. I. ZAMARAEV (*Russia*)
Vice-President: A. E. FISCHLI (*Switzerland*)
Secretary-General: G. DEN BOEF (*Netherlands*)
Treasurer: J. M. WARD (*UK*)

IUPAC Secretariat

Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK.
Telephone: +44 (1865) 747744. Fax: +44 (1865) 747510. E-mail: iupac@vax.oxford.ac.uk

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Associación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Österreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Schweizerisches Komitee für Chemie **(Switzerland)**
Türkiye Kimya Dernegi **(Turkey)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1995, Vol. 17, No. 1 (January)

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IUPAC

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Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

EDITOR: Jeffrey H. Williams
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Front cover: Professor R. J. P. Williams, Oxford University, delivering a lecture at the RSC as part of the IUPAC 75th anniversary celebrations of November 1994.

Stratospheric Ozone

Supersonic aircraft may pose a lower than expected threat. It had been widely believed for almost twenty years that the exhaust gases from supersonic aircraft were one of the great threats to the atmospheric ozone layer. However, new data collected by a team of atmospheric chemists indicate that radicals containing nitrogen atoms, e.g. NO and NO_2, which are derived from jet exhaust gases are not the powerful threat to the lower stratospheric ozone layer that they had previously been thought to be.

These results, published in *Science* **266**, 398 (1994), were taken by 18 scientists working from a number of research groups in several laboratories and consist of measurements taken during last year's Stratospheric Photochemistry, Aerosols & Dynamics Expedition (SPADE), sponsored by the National Aeronautic & Space Administration (NASA). This project is a major annual undertaking where an instrument laden ER-2 aircraft flies out from Mountain View, California, in May, to map the chemical composition of the lower stratosphere. It is part of NASA's on going USD500 million High Speed Research Program, aimed at determining the feasibility of designing an environmentally friendly supersonic aircraft for the 21st Century.

The key issue in such new aircraft is the same problem posed by the Anglo-French Concorde in the early 1970s, namely, the effect of the planes' nitrogen radical emissions on the ozone layer through which the plane flies. In the stratosphere, nitric oxide and nitrogen dioxide take part in complex catalytic reaction cycles that were previously thought to be the dominant process for ozone destruction throughout most of the lower stratosphere. Consequently, the greater the number of aircraft travelling through the ozone layer the greater the destruction.

The recent SPADE measurements reveal however, that in the lower stratosphere (16–20 km above sea level) the effect of nitrogen oxides on ozone is far outweighed by the ozone destroying reactions of hydrogen containing radicals, hydroxyl (OH) and hydroperoxyl (HO_2) and the halogen containing radicals such as chlorine monoxide (ClO) and bromine monoxide (BrO). Small additions of nitrogen radicals at those altitudes actually decreases the loss of ozone because the nitrogen containing radicals react with the hydrogen and halogen containing radicals thereby short circuiting their destructive effect. However, the impact on total ozone concentrations is uncertain due to the complexity of circulation and mixing models in the stratosphere.

Central to these new insights into nitrogen radical chemistry in the lower stratosphere are simultaneous measurements of the concentrations of all of the families of radicals that are involved in ozone destruction. A new instrument developed by Prof. James G. Anderson, Harvard, USA, allowed the first ever comprehensive measurements of OH and HO_2 radicals. The other research groups in the team contributed measurements of the other radicals present in the atmosphere.

Briefly, air is brought into the nose of the aircraft through a flow system designed to provide boundary-layer-free sampling. The [OH] is measured by laser-induced fluorescence using the $Q_1(2)$ and $Q_{21}(2)$ rotational lines of the $A^2(v = 1) \leftarrow X^2(v = 0)$ electronic transition near 282 nm. Collisions with air quench the vibration in the excited state and red-shift the fluorescence to about 308 nm. The absolute experimental uncertainty is estimated to be about 20%. The [HO_2] is measured after chemical conversion to OH by the fast gas-phase reaction with NO. Absolute uncertainties in the [HO_2] which arise from a calibration are estimated at 25%.

In contrast to earlier models that predicted a much more important role for NO_x catalysis, the cycles:

$$NO + O_3 \rightarrow NO_2 + O_2$$
$$NO_2 + O \rightarrow NO + O_2$$

Net: $O_3 + O \rightarrow 2O_2$

and

$$NO + O_3 \rightarrow NO_2 + O_2$$
$$NO_2 + O_3 \rightarrow NO_3 + O_2$$
$$NO_3 + \text{light} \rightarrow NO + O_2$$

Net: $2O_3 \rightarrow 3O_2$

account for less than 20% of the total ozone loss. Oxygen atom densities were calculated assuming a steady state.

As a result of the enormous quantity of halocarbons dumped into the atmosphere over the last few decades, nearly one-third of the photochemical loss of ozone is due to reactions involving ClO and BrO radicals. The most important processes are:

$HO_2 + ZO \rightarrow HOZ + O_2$
$HOZ + light \rightarrow OH + Z$
$Z + O_3 \rightarrow ZO + O_2$
$OH + O_3 \rightarrow HO_2 + O_2$

Net: $2O_3 \rightarrow 3O_2$

where Z = Cl accounts for about 30% of halogen controlled loss and Z = Br accounts for between 20 and 30%. The reaction set

$BrO + ClO \rightarrow Br + Cl + O_2$
$Br + O_3 \rightarrow BrO + O_2$
$Cl + O_3 \rightarrow ClO + O_2$

Net: $2O_3 \rightarrow 3O_2$

is responsible for 20–25% of the halogen controlled loss. Finally,

$O + ClO \rightarrow Cl + O_2$
$Cl + O_3 \rightarrow ClO + O_2$

Net: $O + O_3 \rightarrow 2O_2$

accounts for 5% of ozone loss by halogen chemistry at 15 km a.s.l., increasing to 25% at 21 km a.s.l. The formation of $ClONO_2$ and $BrONO_2$ leads to ozone loss through photolysis of NO_3 followed by the above reaction. These processes account for 10–15% of the halogen controlled loss rates.

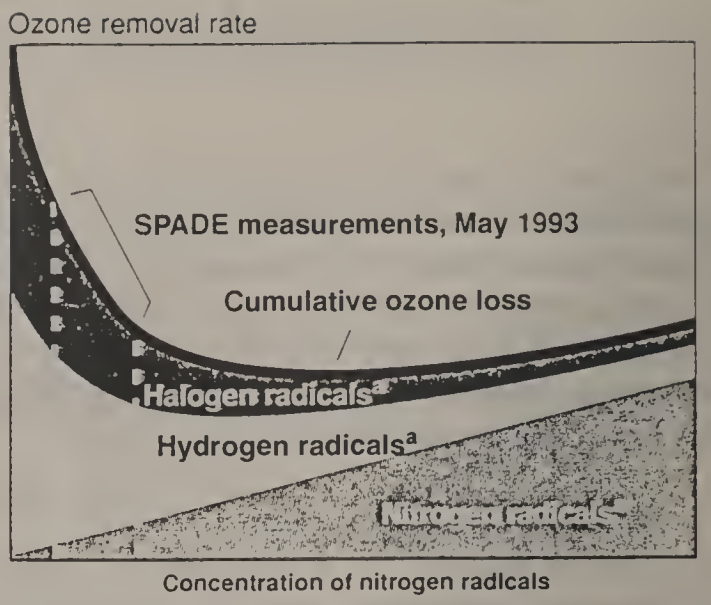
In a recent study (Susan Solomon *et al.* Boulder, USA, *J. Geophys. Res.*, **99**, 20491 (1994)), it has been suggested that to fully understand the details of the ozone balance at altitudes below 20 km one may well have to include reactions involving iodine. The investigation into iodine reactions was sparked by considerations of the fate of CF_3I, a potential replacement for ozone-depleting halons used in fighting fires. The authors stress, however, that the iodine released form CF_3I by sunlight photolysis is unlikely to be involved in ozone depletion by direct reaction, but rather by acting as a facilitator to make chlorine and bromine more potent. As shown in this sequence of reactions, with Z being Cl or Br;

$Z + O_3 \rightarrow ZO + O_2$
$I + O_3 \rightarrow IO + O_2$
$ZO + IO \rightarrow Z + I + O_2$

Net: $2O_3 \rightarrow 3O_2$

The photolytic production of ozone from molecular oxygen, by light at wavelengths < 200nm, exceeds photochemical loss at all latitudes below 45°N during May.

These mainly spectroscopic measurements are generally held to be some of the most complete and spectacular made in experimental atmospheric physical chemistry. A number of scientists are now proposing that this particular level in the atmosphere may be suitable as a corridor for supersonic air traffic with minimum damage to the all-important ozone layer. In the middle and upper stratosphere, however, the nitrogen containing radicals are still by far the most important ozone destroying molecules.



Data suggest complex role of nitrogen radicals in ozone depletion. Because of complex interactions among the halogen, hydrogen, and nitrogen radical – all of which can catalyse ozone destruction in the stratosphere – the rate of ozone removal responds nonlinearly to changes in the concentration of nitrogen radicals. In the lower stratosphere, where abundances of all the radical families were measured during the 1993 Stratospheric Photochemistry, Aerosols & Dynamics (SPADE), increases in the concentration of nitrogen radicals would actually result in a decrease in ozone loss.

Of course, the ozone hole over Antarctica is still there and any changes to the flight paths of supersonic jet aircraft will affect it only slightly. The various fluorocarbons which have been pumped out into the atmosphere are to a large extent still there and when the sunlight hits them in the stratosphere over Antarctica, an ozone hole develops.

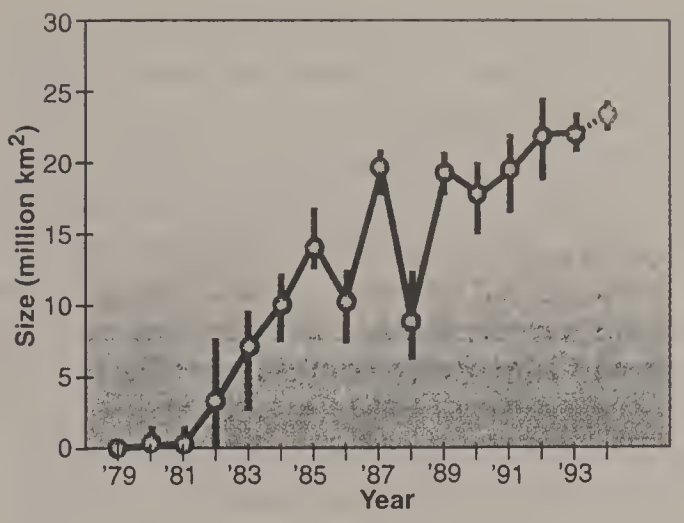
Researchers had expected that the record ozone loss of 1993 would not be repeated. The huge amount of volcanic ash thrown out by Mount Pinatubo in 1991, which enhanced the chemical destruction of ozone, is now almost gone from the atmosphere. The microscopic debris from the volcano provided sites for reactions which destroy ozone. However, instead of recovering this year, after most of the volcanic ash had gone, the ozone hole over the southern continent is almost as wide and as deep as ever. The graph shows the area of the annual variation in size of the ozone hole over Antarctica (*Science* **266**, 217 (1994)).

The most alarming possibility for this continuing disappearance of ozone from the Antarctic sky is that the ozone hole has recovered as much as it will from the ash of Mount Pinatubo, and that the hole is being deepened and enlarged by the steady increase of chlorine and bromine from synthetic chemicals.

International controls on the emission of fluorocarbons into the atmosphere are expected to halt the increase in the concentration of Cl and Br in the stratosphere after 1998. In recent years, however, the chlorine levels have been increasing at the rate of a couple of percent per year. That may have been enough to extend ozone destruction beyond the thin layer where major losses were confined before Pinatubo's eruption. If those bonds have been breached, it might take several years before scientists start monitoring a levelling off of ozone destruction.

The subject of atmospheric chemistry is also of great current interest to nonscientific organizations. Munich Re, the world's largest reinsurance company, has called on governments to meet their commitments to stabilizing 'greenhouse' gas emissions in line with the world climate convention, signed in Rio de Janeiro in 1992, because of threats to the world's climate. The company is becoming convinced that there is a trend towards more frequent and more severe natural disasters arising from changes to the world's climate.

Apparently, a number of insurance companies are increasingly worried that global warming may be responsible for a recent sharp increase in insurance claims resulting from natural disasters, which have resulted in several bankruptcies in the insurance industry.



Annual variation in the area of the ozone hole over Antarctica. The unit of ozone concentration is the Dobson, values today are of order 100 Dobsons, whereas as in the late 1970s, before the hole began to form, they were typically 280 Dobsons. (Figure taken from *Science*).

In addition to Munich Re, a number of other major insurance and reinsurance companies, together with several international banks, are also becoming involved in the global warming debate. But, as yet, are not committing themselves to specific policy changes, despite pressure from environmental groups to take steps to help shift energy policy away from fossil fuels.

Mode Selective Chemistry

One of the early uses by research chemists of the laser was as a source of monochromatic light. Previously, it had been necessary to disperse a white-light source to obtain monochromatic light, however, for a limited range of wavelengths this was no longer necessary with lasers. With time, additional uses of the laser were discovered, for example, when tuneable lasers became routinely available the field of molecular spectroscopy was revolutionized.

As lasers increased in sophistication and reliability, it became possible to measure a molecular transition with ever increasing precision. Indeed, the point arrived when the field of ultra-high-resolution molecular spectroscopy was born, the measurement of line widths to an accuracy of better than 1 in 10^8. Interestingly, one of the great chemical spectroscopists, Prof. Robert Field (MIT, USA) asked at this time that perhaps we were losing sight of the interesting science in the accumulation of decimal points – we should exchange decimals for concepts.

In most small molecules there is likely only to be one chromophore, that is, the part of the molecule, perhaps a bond where the charge cloud is able to come into resonance with incident radiation, which is actually absorbing the laser radiation. The observation that energy, of order, a visible photon (a couple of electron volts) could be selectively placed in one particular bond in a molecule soon lead to the idea of bond-selective chemistry. That is, that activation of one bond might under appropriate conditions lead to increased chemical activity of that bond. For example, if the absorbing molecule was involved in a chemical reaction involving a bond breaking process, if sufficient energy could be put into one part of the molecule, perhaps that part nearest the centre of bond fissuring, then the reaction rate might be influenced by the presence of the laser light.

Unfortunately, early promise soon gave way to disappointment. As lasers developed, it became possible to produce shorter and shorter laser pulses, the limit to-

day are pulses of a few femtoseconds (10^{-15} of a second) – a few fringes of light, which are more rapid than the rate at which energy moves from one bond to another bond within a molecule. These studies clearly showed that even though one bond might initially absorb a photon, this energy was redistributed within the other bonds of the molecule on a time scale fast when compared to the rate of the various chemical reactions. Consequently, there was no bond-selective effect of laser light on chemical reactions. The effects that had been observed were more likely to be the effect of thermal heating of the gas sample caused by absorption and then thermalization by molecular collision, increasing the observed reaction rate. In effect, there was no more specificity induced by the laser than would have been found by simply heating the gas with an ordinary Bunsen burner.

Such disappointments do not, of course, deter everybody. Indeed, they can act as a spur for further investigation. The goal of being able to use precisely tuned laser light to control the outcome of a chemical reaction is too seductive to be ignored for long. Indeed, the idea of using a laser like a molecular-scale scalpel was so seductive that the magazine *Fortune* ran a story in 1977 entitled 'Laser Alchemy is Just Around the Corner.' It said chemists would soon be fashioning new fuel, drug molecules and detergents at will.

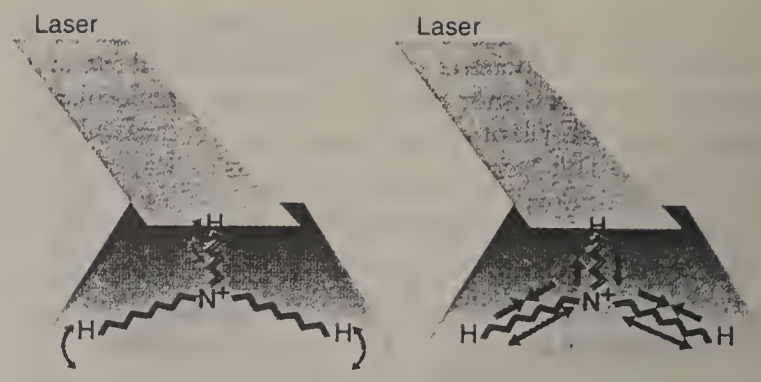
Early in 1994, Prof. Scott L. Anderson, State University of New York, Stony Brook, USA, and his colleagues reported that the reaction of acetylene cations with neutral methane could be strongly influenced by excitation of the bending vibrational mode of $C_2H_2^+$ (*J. Chem. Phys.* **101**, 5410 (1994)). Now Prof. Richard Zare, Stanford University, California, USA, and colleagues report that excitation of the 'umbrella' mode of the ammonium ion exerts a strong influence on the rate of reaction of that ion with ND_3 (Science **266**, 259 (1994)).

The reaction studied by Anderson *et al.* is

$$C_2H_2^+ + CH_4 \rightarrow C_2H_3^+ + CH_3$$

where excitation of the bending mode of the acetylene cation increased the rate of reaction by a factor 30. In contrast, excitation of the carbon-carbon stretching vibration had little effect on the rate. This is surprising, as the bending vibration involves a bond (C–C) that is not broken during the reaction. Anderson suggests that it is the amplitude of motion of the terminal H atoms which drives the reaction. A low frequency bending motion causes the H atoms to execute large amplitude motions. This is what is required for reaction, as the hybridization of the C atom must change from sp to sp^2, which has 120° bond angles. Bending motion is just what is required to drive the acetylene molecule into the appropriate reactive configuration.

In the ion-molecule reaction studied by Zare *et al.* NH_3^+ react with its deuterated analogue ND_3. Three outcomes are possible: deuterium abstraction yielding NH_3D^+ and ND_2; charge transfer to form NH_3 and ND_3^+; and proton transfer yielding NH_2 and ND_3H^+. The researchers prepared the ion reagents in two isoenergetic vibrational states of different combinations of bending and breathing motions; they found that the bending motion enhances charge transfer and deuterium abstraction and hinders proton transfer.



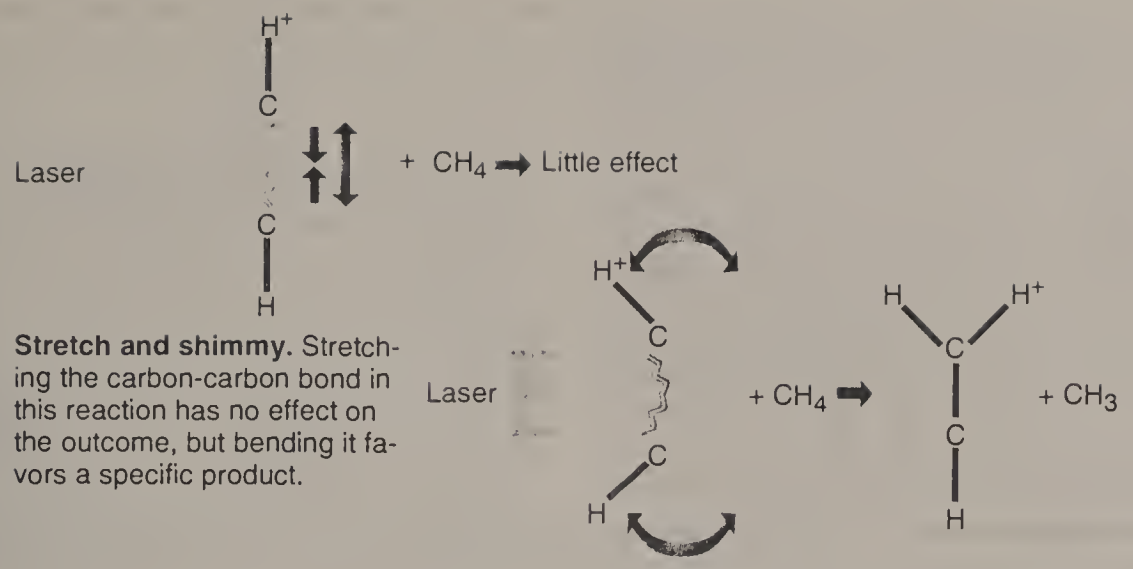
Shake it up. Only the 'umbrella mode' vibration (left) of an ammonia ion affects its reaction course; the 'breathing mode' (right) has no effect.

The 'umbrella' mode of the ammonium ion turns the molecule inside out, like an umbrella in a strong wind. The breathing motion stretches and contracts bonds along the N–H axis axes in unison. Zare *et al.* prepared the ion in two different vibrational states, but of the same total energy; one possessing 1 quantum of breathing vibrational energy and 2 quanta of umbrella bending, giving a total energy above the ground state of 0.63 eV; the other prepared state had no breathing quanta, but 5 quanta of bending motion, giving a total vibration energy above the ground sate of 0.6 eV.

It was found that the reaction rate is strongly influenced by the bending or umbrella motion of the NH_3^+, but is insensitive to the breathing vibrational motion. Strongly suggesting mode-selectivity.

Zare notes that these experiments directly address the question of whether it is the total vibrational energy, above the ground state, or the type of vibrational motion which influences the rate of reaction.

It is likely that these experiments will lead to a rapid rise of interest in this field, which could well be set to fundamentally change our picture of chemical reactivity. Most chemistry is done by 'shaking and baking', one mixes the reactants, heats the system, and extracts the products. In many cases, heat is produced which may push a reaction along several different paths at the same time – one that produces the desired product, and others, perhaps the majority, which produce nothing of interest. However, if it becomes possible to nudge the chemical reactivity of particular bonds in a molecule, the reactants might well follow only a limited number of pathways, thereby eliminating waste and the possible production of unwanted products.



Stretch and shimmy. Stretching the carbon-carbon bond in this reaction has no effect on the outcome, but bending it favors a specific product.

Now that it has been shown to be possible, even in only two chemical reactions, to use a laser to influence directly the product distribution of the reaction, chemists would like to generalize this procedure. However, what of the problem of localizing the laser excitation sufficiently long to influence the reaction?

The concept of 'active control' has now been put forward to control the excitations of the probe molecule. Laser pulses delivered during the reaction itself would coax the molecule along a desired path by making the molecule move in new and, for it, unnatural ways.

To achieve this coaxing, a series of laser pulses carefully timed and modulated so that they match the bending and stretching motion of the individual bonds is incident upon the probe molecule. Consider the molecule HOD, a first pulse sets the two bonds stretching and contracting at different rates. A second pulse would then be delivered at just the right moment to catch the HO bond as it starts to contract and the DO bond as it starts to stretch. The result; the hydrogen careens back while the deuterium is kicked further out, making that bond more susceptible to rupture.

Theoreticians are now convinced that this is a possible way of controlling and directing whole reactions. Prof. Herschel Rabitz, Princeton, USA, is trying to determine the best experimental shape for such laser pulses, using a process which his colleagues term 'obedience training for molecules.'

The first pulse sets the molecule in motion and the second can be used to explore the extent of the induced motion. Like an unruly dog, the molecule quickly teaches its handler the best way of influencing its behaviour. The pulses are very narrow and are generated at very high frequencies, one may envisage doing millions of experiments in an hour.

Bringing Chemistry to Life

R. J. P. Williams

As part of the 75th anniversary of IUPAC, Prof. R. J. P. Williams of the Inorganic Chemistry Laboratory, University of Oxford, was invited to deliver a lecture, entitled *Bringing Chemistry to Life*, at the Royal Society of Chemistry, London, in November 1994.

I thought it appropriate to use the title 'Bringing Chemistry to Life' to show how recent advances in different areas of chemistry are coming together to give us a new view of the nature of many objects around us, including living organisms. An understanding of this chemistry must lead us to revalue our approaches to teaching and research in chemistry.

The subjects which I wish to integrate are geochemistry, inorganic and organic (especially bio-organic) chemistry and biological chemistry. All chemists know the nature of the first three, but biological chemistry is different in one major aspect, it concerns organization. While a chemist concerns himself with structure, and the balance between structural order and disorder, with kinetics of change and with physical and chemical properties it is rare for him to look at flow, a requisite of organization. Organization is usually left to the chemical engineer but in fact all the operations of chemistry in a research laboratory are organized in a flow sequence. There are three major advances which are allowing a constant stream of new chemical products. The first two are

- the exploitation of a whole range of new catalysts;
- the use of new selective carriers for fragments during synthesis.

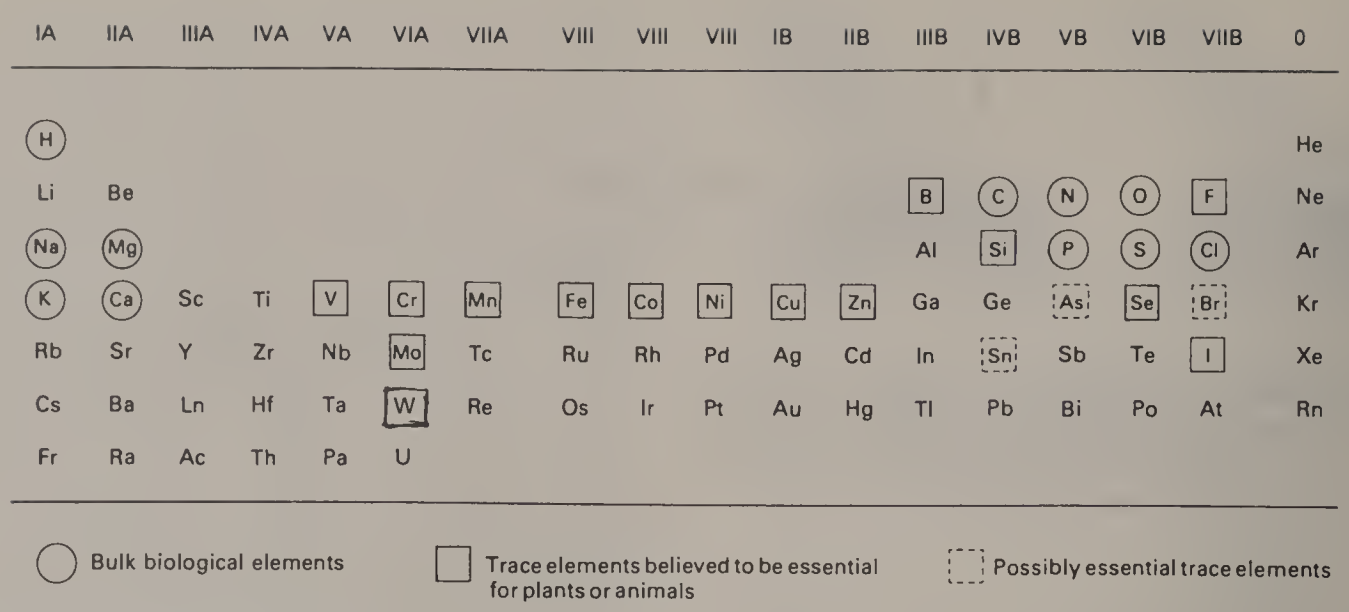

IA IIA IIIA IVA VA VIA VIIA VIII VIII VIII IB IIB IIIB IVB VB VIB VIIB 0
H He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Ln Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra Ac Th Pa U
Bulk biological elements
Trace elements believed to be essential for plants or animals
Possibly essential trace elements

Fig. 1 The Elements essential for Life.

Outstanding here has been the expansion of organic chemistry using a vast armoury of inorganic elements ranging in the Periodic Table from lithium to thorium. This marriage of organic with inorganic chemistry has produced, as one result, organometallic chemistry. The third area is

- The study of organic molecules related to, or extracted from, biological systems from small units to DNA with special stress on understanding proteins. This is called bio-organic chemistry and here there is overlap with biochemistry and biological chemistry.

Of importance here is the advance in bio-inorganic chemistry. It is bio-inorganic chemistry that I shall use as a starting point for the discussion of 'Bringing Chemistry to Life', a title which clearly has a literal and a metaphorical sense. Bio-inorganic like bio-organic chemistry is the study of molecules related to (often called models) or extracted from biological systems, but now containing an inorganic element in addition to H, C, N, O, P and S. The first major advance here is the clear knowledge that life is not just some form of 'organic' chemistry.

The elements of life and the periodic table

We all accept that H, C, N and O, the elements of organic chemistry, plus a little P and S are essentially the stuff we are made. Figure 1 stresses this. Analysis shows that all life, while requiring these six elements demands more than ten other elements of the series; Na, K, Mg, Ca, (B), (V), Mo, Mn, Fe, Co, Ni, Cu, Zn, Si, Se, Cl. In fact we do not know any life which exists without ten of these elements, and we know some living systems which require more remote elements such as Sr, Ba, W. I. A look at this list shows that almost every group of the Periodic table has a representative in all life. Referring back to the recent development of organic chemistry, we notice that use of many elements, like the use of many elements in life, is to take advantage of the fact that the Periodic Groups are groups of elements with separate functional value. There is a distinction however, between value in life, and in organic chemistry, since the first is value in a flow system in water and must use readily available elements, while the second is value in synthesis in organic solvents and can exploit any of 90 elements. Given this difference, the underlying reason for using elements from seventeen different groups of the Periodic Table is that this optimises all possible functional values. Living organisms developed spontaneously some 4×10^9 years ago from a mixture of the seventeen groups of elements in the sea.

The uses of elements in life

The immediate question is what are the functions which life required which makes these 15–20 elements so valuable. Taking first the need to make polymers we note the basic 'organic' chemical elements, H, C, N and O, make the best polymers with kinetic stability. However, we also observe that making polymers requires a confined space, a chemical apparatus which in biology is a cell with a membrane (Fig. 2). The membrane also effectively made from the same four elements. The need for P and S is seen if we remember that all organic chemistry requires not only confinement in a vessel, but (i) catalysts and (ii) reactive carriers of fragments for synthesis. Both the carrier and the fragment need to be more reactive than the C/H/N/O product polymer. In the transfer of fragments P, in phosphate esters or anhydrides, and S, in thiols or thio-ethers, are more reactive than the vast range of organic molecules. Moreover, an RS^- base is a good catalyst for acid/base reactions. It is a general feature of the Periodic Table that kinetic stability decreases down a group when transfer and catalytic properties improve. In passing, note the deliberate weakness of DNA and RNA as phosphate diesters which is an essential feature of their character and

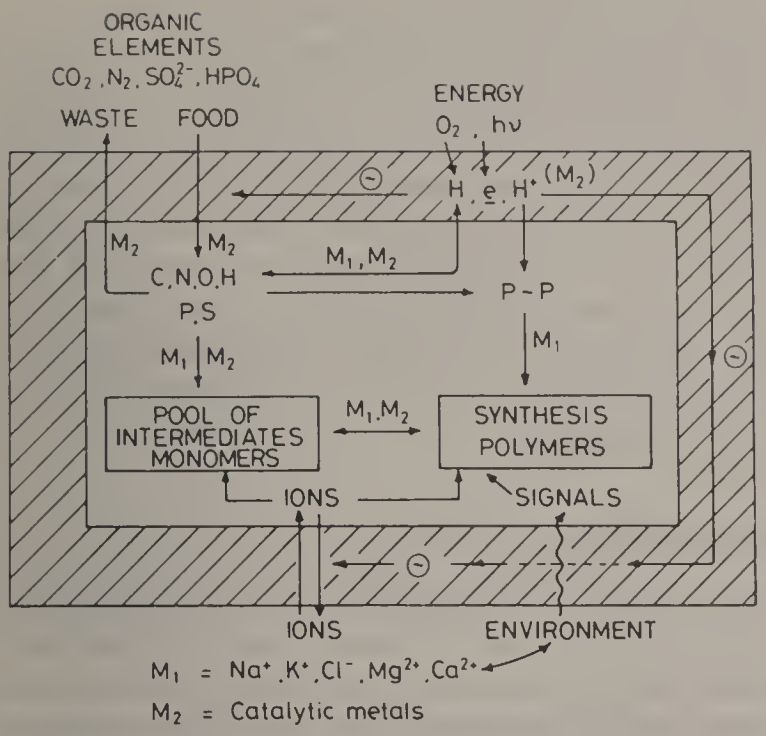


Fig. 2 An outline of a living cell's functional use of elements. In primitive conditions O_2 was not available.

which is absent from proteins.

Turning to the other elements, let us consider next the least reactive. Why does a biological system need Na^+, K^+ and Cl^- which do nothing chemically? The answer is simple – organic chemistry in water (life's chemistry) is the chemistry of organic anions in a weak containing vessel. These chemicals create an uncompensated osmotic (mechanical), and an uncompensated charge (electrical), field which would burst the cell membrane. To balance the two fields in the sodium chloride sea, the primitive cell had to export Na^+ and Cl^- and accept the minority K^+. There was no other possibility. Moreover, the anions are open to precipitation by the Ca^2 of the sea, so it also had to be expelled (Fig. 2), the Mg^{2+} was useful as a mild catalyst for anionic reactions. Virtually all phosphate transfers in organisms are managed by controlled Mg^{2+} Lewis acid catalysis. The calcium outside the cell wall and is used to form complex stabilising structures and supporting shells of $CaCO_3$. Suddenly, we observe the parallel with geochemistry. Summarizing, there could be no life without handling the essential elements H, C, N, O, P, S, Na, K, Mg, Ca and Cl, since they dominate and always dominated our environment, especially the sea. Life could not choose the environment, but the environment forces choice on living forms.

Oxidation and reduction

The observant reader will have noticed that the chemistry I have described so far is acid–base chemistry. Proteins and fats can be made by acid–base catalysed reactions provided there are acid base catalysts (Mg^{2+}, H^+ and RS^-) and carriers (P and S compounds), and so long as the starting materials are in the correct oxidation states. Thus organic chemists do not start syntheses from CH_4, O_2, N_2, H_2O, but from carbon, nitrogen and oxygen in particular oxidation states such as organic compounds. To go from the raw material of geochemical interest, oil (gas, CH_4), water and the atmosphere (N_2) there has to be redox chemistry. Once again the problem is how to choose catalysts and carriers of fragments for this chemistry. While S can be so used with difficulty as a catalyst in redox reactions, chemistry tells you that this is where transition metal chemistry is at its best. The most abundant transition metals are, and were when Earth formed, Fe and Ni and they, with Mn, Co and Mo (W), would have been available in the sea under the early reducing conditions. These are the elements which readily undergo valency changes so that they are sensitive to an oxygen atmosphere. Fortunately, the early Earth had no O_2 and lots of Fe^{2+} and a few other metals such as Ni^{2+} and $Mo(MoS_4^{2-})$. Thus biological systems on early Earth could make use of not just any sulphides (compare organo-metallic phosphines), but especially iron, nickel and molybdenum sulphides. The consequences are striking. The earliest known organism, the archaebacteria, use as well as the eleven elements listed above, the elements Fe, Co, Ni and Mo (or W) in redox chemistry. Even today, little of life's chemistry succeeds without Fe/S and Mo/S compounds. (Biological systems could not utilize the diversity of today's organometallic chemistry since the compounds are not stable in water). We observe today (in proteins):

- no nitrogen is fixed without molybdenum;
- very little C/H/O redox chemistry proceeds without iron.

More selective redox chemistry, whether organic or in biology, demands a greater variety of catalysts and carriers. They appeared in primitive nature: Co(vitamin B_{12}), Ni(F-430), Mo(Mo-pterin), Fe(haem). Thus in the inert early atmosphere, anaerobic biology evolved using, at least, fifteen elements. We know of no other early life. It then made one serious mistake which concerns sources of hydrogen and sources of energy. We have excluded from discussion so far any chemistry of Cu or Zn which due to the insolubility of their sulphides would have been of low availability 4×10^9 years ago.

Sources of hydrogen

The readily available source of carbon has always been CO_2 since it is more soluble in water then CH_4. Starting from the water soluble CO_2, the needs for making organic compounds are sources of hydrogen and energy. Undoubtedly, H_2S and Fe/S compounds would have been the first source of both, but at some early period (3×10^9 years ago) the bountiful supply of H_2O became the donor of H for CO_2 conversion to C/H/O molecules

using light. The fortunate feature was that the energy of visible light is sufficient for the purpose of splitting H_2O to $H_2 + O_2$. The unfortunate feature for anaerobic life is that the second product is O_2. Dioxygen is an extremely dangerous compound for C/H/O molecules, especially in the presence of trace element catalysts. The interaction of O_2 with the surface waters raised the redox potential only slowly due to redox buffering by the reducing surface waters. Worse was to follow for anaerobic life, as dioxygen (unstable) accumulated in the atmosphere. In turn, sulphide went to sulphate, ammonia to dinitrogen, thiomolybdate to molybdate and Fe^{2+} (iron) was lost as precipitated $Fe(OH)_3$. Even worse was to follow from this organic chemical greed for hydrogen since slowly after the removable of sulphide, dioxygen removed selenide (a hydrogenation catalyst) as selanate, iodide became available as poisonous iodine and the removal of sulphide not only increased the concentration of poisonous zinc, but finally introduced the extremely poisonous metal, copper. There was but one way forward – turning all the new trace elements in turn into new catalysts or control devices. Much as new catalysts and carriers advance man's organic chemistry today, so they advanced biological evolution in aerobic organisms.

The fuels of biology

Once light could be used to reduce CO_2, and at the same time liberate O_2, a new possibility arose for producing energy. The reduced carbon, C/H/O compounds, could be re-oxidized to CO_2 and H_2O generating energy. This development of a fuel cell from O_2 + reduced carbon allowed life to escape from a static (plant-like) existence to a mobile animal-like scavenger condition, even at the unicellular level, some 2×10^9 years ago. The very fact that this oxidation could not be effective as a source of energy until the partial pressure of O_2 rose to be quite high meant that enormous quantities of early plant material, from H_2O and CO_2 degraded as C/H/O compounds, finished as the stores of oil, coal and gas, which man is now dissipating (with O_2) since he is over greedy not for hydrogen, but for energy.

Evolution

With both new catalysts and new fuels for energy, instead of evolution driving the environment the opposite occurred. The new environment allowed new organic chemical developments. This is oxidative chemistry using oxidizing agents such as O_2. Provided that the inner metabolism of the cell could be maintained in a reducing medium, essential for production of proteins, fats and DNA (RNA), the external oxidizing medium could be used with the new catalysts (especially Cu not Fe which was largely lost) to generate new stable polymers outside the cell, connective tissue of sufficient strength and rigidity to give multicellular organisms. The required chemistry is oxidative cross-linking of polymers by radical reactions. The manipulation of these strong connective tissues during growth also required the actions of hydrolytic enzymes using the newly available strong Lewis acid, Zn. Thus copper and zinc (released from sulphides by dioxygen) together with dioxygen generated multicellular life some 2 to 1×10^9 years ago.

Organization

It is when cells come together that biological organization (the new feature in chemistry which biology introduces) is seen so strikingly as controlled flow of energy and material. This organization has structure through the connective tissue, but it can only be maintained by pumping (energy) and internal messages in nerves and in the blood stream, and by co-operative action of sensing devices and muscles in animals to allow scavenging. In many message systems, the extra-ordinary developments are dependent on inorganic elements alone – the $Na^+/K^+/Cl^-/Ca^{2+}$ messages in nerves and muscles. They are equalled by the development of organic messengers, hormones and transmitters, in the extra-cellular fluids. Most frequently, the new compounds are based on syntheses (secondary metabolism) using oxidation by the new inorganic catalysts – steroids, thyroxines, prostaglandins and so on, or on new peptides often released by zinc enzymes. Thus evolution is seen to be driven by the changed availability of elements which was the result of a mistake by life – the drive for hydrocarbon of anaerobes which unleashed dioxygen and in turn generated a new sea of poisonous trace elements. We must discover the mechanism of the link between environment change and DNA changes. Is it by 'directed' mutation?

Today, man changes the environment through his industry which in effect uses new chemical methods of high temperature to make new materials from previously little used or differently used elements. Will he slowly force change, not just on the atmosphere, but on DNA through trace element changes in the sea over hundreds, thousands, even millions of years? Figure 3 is an attempt to put man's chemistry in an historical and biological perspective.

Surveying chemistry today

I have tried to sketch the interactive nature of geochemistry, organic and inorganic chemistry, in both life and by implication in industry. There are obvious risks in what man is doing in that he is expanding the range of available chemical elements. This expansion

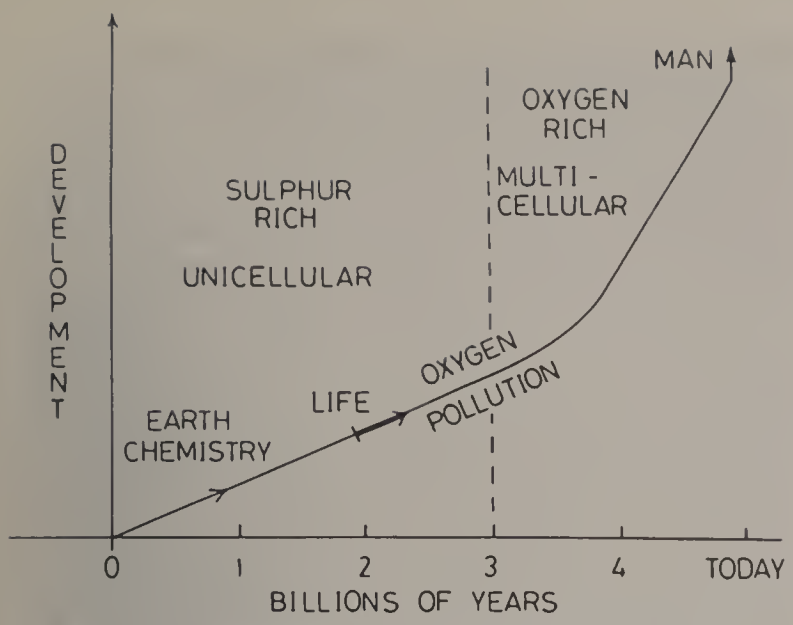


Fig. 3 The development of chemistry and life seen as increasing complexity of order and organization.

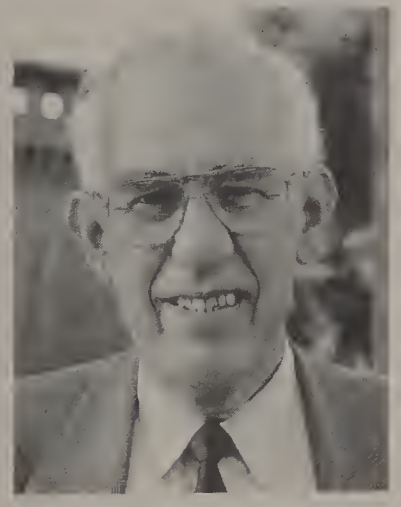
has happened once before extending over two billion years when O_2 generated by early life changed chemistry of the ocean and totally altered evolution, largely through changes in catalysts and carriers. Catalysts and carriers dominate organic chemistry. Today, there is a difference in that man is self-conscious and aware. He can then remove risks, but he has to be willing to take precautions. It is for the chemist to teach not just chemistry, but its risks and proper uses since only the chemist can show the nature of life in the context of materials in the environment.

The subject matter in this lecture will appear in a book form in 1995. The Natural Selection of the Chemical Elements, *R. J. P. Williams and J. R. R. Frausto da Silva, Oxford University Press.*

Secretary General's Column

Gerrit den Boef

The year 1994, has not been uneventful. A particular success of 1994 has been the fruitful co-operation between UNESCO and IUPAC. In January 1994, a UNESCO–IUPAC Co-ordinating Council for Chemistry (CCC) was created. This committee will be the vehicle through which future joint activities, between the Union and UNESCO, will be conducted.



Gerrit den Boef

UNESCO will assist in running our CHEMRAWN programme, as well as supporting projects to be carried out by the Division in those areas which are considered to be of high priority by UNESCO. Such high-priority areas include: the needs of least developed countries, rural areas and women. Already in the 1994–95 biennial budget of UNESCO, funding has been made available for a few projects to be carried out by IUPAC in 1995. These projects are:

Clinical Laboratory Improvement Program for Kenya, submitted by Clinical Chemistry Division, IUPAC.

Training Program for the Establishment of a Seafood Safety Monitoring Program for Cigutera, submitted by the Commission of Food Chemistry, IUPAC.

Training Program for the Establishment of a Food Safety Monitoring Program for Mycotoxins (Ochratoxins), submitted by the Commission on Food Chemistry, IUPAC.

At the recent CCC meeting in December 1994, the planning of the IUPAC input in the framework of the 1996–97 UNESCO budget has started. The co-operation also includes a training programme for safety and environmental protection in chemical production in which the IUPAC partner is COCI.

There is an evident interest on the part of UNESCO to increase our joint endeavours. This desire for closer collaboration has been expressed by the Director General of UNESCO, Frederico Major, in a meeting with our Vice-President Prof. Albert Fischli, as well as by the Deputy Director General Dr Badran in a meeting with myself. We have great expectations of our collaboration with UNESCO.

At the Bureau meeting in September many items of topical interest were discussed. Remarks on a few of them are included in this column.

Names and symbols of the transfermium elements

Since they were made known, numerous enquiries have been received about, and reactions expressed to, the recommendations by the Commission on Nomen-

clature of Inorganic Chemistry (II. 2/CNIC) on names and symbols of the transfermium elements [*Pure Appl. Chem.* **66**, 2419–2421 (1994)].

In order to avoid any misunderstanding on the way in which the recommendations were dealt with by the Bureau, we feel that it is appropriate to inform the chemical community by means of the minutes of the Bureau meeting (Antwerp, September 1994) on this agenda item.

These minutes have been approved by the Officers of the Union then present, but they are still subject to approval by the Bureau when it meets next (Guildford, August 1995) at the 38th IUPAC General Assembly.

The minutes read as follows:

'Prof. Komarek referred briefly to the long standing problem for IUPAC of recommendations on names and symbols for the transfermium elements. Interim systematic names and symbols had been recommended (1979), and a Transfermium Working Group (TWG) set up (1986) under the joint auspices of IUPAC and International Union of Pure and Applied Physics (IUPAP). The TWG's conclusions on criteria that must be satisfied for the discovery of a new chemical element to be recognized and on discovery of the transfermium elements, were duly endorsed by the two Unions and published by IUPAC in *PAC* (1991 and 1993). He emphasized that, after detailed examination of all the criticisms from Berkeley, TWG did not find it necessary in any way to change the conclusions reached.

Accordingly, President Zamaraev had requested the Commission on Nomenclature of Inorganic Chemistry to consider the conclusions at its meeting in 1994 (Balatonfüred 31.8.94–3.9.94). This had been done, and the outcome was available as a late paper to the Bureau. Prof. Komarek noted the wide spread of national representations at the meeting, the significant vote that an element should not be named after a living person, the sensitivity of the Commission to the suggestions of the three laboratories involved in the choices for names, and the remarkable consensus in the carefully administered voting in respect of the name for each element. In view of the lack of agreement over some thirty years by the relevant laboratories, he proposed acceptance of the Commission's recommendations on names and symbols for the transfermium elements by the Bureau, preferring to send them to Interdivisional Committee on Nomenclature and Symbols (IDCNS) for definitive publication in *Pure & Applied Chemistry* and simultaneous release to national chemistry news journals, rather than to send them to the laboratories involved and chemical societies worldwide for comment as suggested by the Commission.

Prof. Brown pointed out that the recently propose name 'seaborgium' for element 106 had been accepted by the American Chemical Society nomenclature committee. After due deliberation, Prof. Komarek's proposal was accepted unanimously by the Bureau.'

Understandably, the Chairman of CNIC, Prof. A. M. Sargeson, is concerned by some of the recent criticism, especially as he feels this is due to mis-information. He has therefore prepared the following statement to demonstrate how carefully the issue was conducted.

'Recently, the Inorganic Nomenclature Commission was charged by the Bureau of IUPAC to name the transfermium elements. The three laboratories concerned had been squabbling for many years about who had discovered which element and what their names should be. The problem was obviously unresolvable by the laboratories concerned, and IUPAC appointed two sets of referees, firstly to apportion credit for the discoveries, and secondly to name the elements. The Transfermium Working Group of IUPAC and IUPAP reported its final conclusions on the discovery issue of IUPAC in 1993, which were endorsed by IUPAC in 1994.

At that point, the Nomenclature Commission accepted the duty of naming the elements, and the Chairman wrote to the laboratories concerned, asking them to suggest names for the elements where discovery was claimed to comment on appropriate names for other elements in the group. The letter also requested reasons for the choice of names. It was pointed out that a likely issue was whether an element should be named after a person, since the Commission had no clear policy on the matter, and that many elements had been named after places and some after their properties or the properties of their salts. It was also suggested that an imaginative attitude for naming an element for posterity was called for, and the views of the laboratories would be welcome. The letter raised the question that, if the Commission did decide not to use the names of individuals for elements, it would be helpful to have the laboratory's preference in such circumstances. All three labs responded, addressing some of the issues raised in the letter, but not all of them, and there many more suggestions for names than there were elements.

At least, the Commission had time to consider the proposals from all three laboratories before meeting in Hungary. Twenty chemists were present, all with equal voting rights, from twelve different countries.

At the beginning of the debate it addressed the precedents for naming elements, and agreed unanimously to continue the practice of naming elements after appropriate places, properties and scientists. However, it resolved that elements, should not be named after a living person. The majority of the Commission (80%) felt it was necessary to have the perspective of history in relation to these discoveries before such a decision was made. As far as the Commission is aware, this was the first time general policy had been established in regard to this problem.

The Commission then agreed to accept the conclusions of the Transfermium Working Group as one of the

bases for selecting names. It was sensitive to suggestions from the three laboratories about the choice of names and, in the final analysis, all of the names chosen came from their proposals, but not necessarily in the order suggested. Clearly, the above policy decisions eliminated some of the suggestions, and there were still more names proposed than elements available to be named. The recommended names were reached after extensive discussion with a remarkable degree of consensus. It must be obvious to everybody that the Commission could not totally satisfy any of the laboratories concerned nor even the members of the Commission itself, given the previous history of conflict regarding this problem. However, nobody could be critical of the names finally chosen in terms of the appropriateness for the area of chemistry.

Some of the problems which have subsequently emerged could have been avoided, if the laboratories concerned had addressed the Chairman's letter more carefully and more fully. It is clear that the Commission approached the problem and dealt with it in a very objective manner from the point of view of chemistry in general, and a number of complaints which have been raised subsequently are certainly not valid. For example, no one from the laboratories concerned addressed the commission at the meeting. However, there were members of the Commission from all three countries involved, Germany, Russia and USA, and it is perfectly clear that those members behaved in an exemplary and objective manner in relation to the decisions that were made. It has been claimed also that elements were named after both Einstein and Fermi in advance of their deaths. As far as the Commission can determine, the names were not even formally proposed until after Einstein's death in April 1955 (see *Phys. Rev. Lett.* 20th June 1955).

The objectivity of the Commission is evident in the choices for the names in relation to people and places, who have contributed significantly to our understanding of the atomic structure, stability and chemistry of the elements. The issue of who discovered which elements is a matter of scientific record and unrelated to nomenclature. It will be known by the relevant scientific community in any event. The fact that some of the names proffered were not chosen at this time does not make than ineligible in the future and, in the situation which the Commission faced, it was inevitable that some of the names had to be chosen in preference to others. It was a responsibility with the Commission accepted and dealt with sincerely and fairly, given the responses from the laboratories concerned, the history in the area, and the relevance of the element names to chemists the world over. '

The present situation is that the Bureau unanimously accepted the proposal by the President of the Inorganic Chemistry Division to publish the recommendations definitively in *PAC*. As the Bureau is the highest authority in hierarchy directed below the Council of IUPAC, there is no possibility to act until the Bureau meets again next August in Guildford. Directly after the Bureau meeting, the Council has to vote on the ratification of the recommendations.

Allocations of the pool of 24 Titular Members

A pool of 24 Titular Member positions was created as a result of the discussions on the restructuring of the scientific activities of the Union in high-priority areas. A number of these positions were given to the Divisions for innovative activities, and others to projects proposed by Bureau members.

The designated projects will start at the General Assembly in Guildford in August 1995. A few example of successful projects requests are:

- Oil Spill Clean-up and Remediation;
- Remediation of Heavy Element Contaminated Sites;
- Polymers and the Environment;
- Environmental Safety Assessment of Agrochemicals.

Divisional structure

Discussions on restructuring the divisional framework were not restricted to the pool allocation. A particularly important point was the discussion of focusing the scientific efforts more in the direction of the role of chemistry in the study of environment, health, materials and biological problems.

The initiative for this discussion had already been made by Division VI at Lisbon and broadened by VIce-President Fischli at the Bureau meeting as a result of his discussion with Division Presidents which formed part of his Vice-Presidential critical assessment. No decisions have as yet been made, but undoubtedly some interesting changes will be proposed at the General Assembly in Guildford later this year.

Chemistry and the environment

A review of the IUPAC activities in environmental chemistry, prepared by Prof. Jack Calvert, was presented and well received by the Bureau. The document will be extended and published.

A number of new activities are about to start, resulting from critical remarks both from outside and inside the Union. It is unlikely that everybody will agree that the restructuring activities are proceeding fast enough, but if we can keep up the present momentum we likely to be successful.

We should remember the wise words of one of my Divisional President colleagues who said, during my time as President of Division V, 'The Union is better served by evolution than by revolution.'

Task Force on Scientific Aspects of the Destruction of Chemical Warfare Agents

Not many years ago, most discussion of the destruction of chemical weapons dealt only with political problems. Moral considerations were often invoked, but the problem was one of nation states who believed that these weapons would somehow protect them and were vital to their self-interest.

In the post-Cold War world, however, we are beginning to achieve a political consensus, exemplified, for example, by the Chemical Weapons Convention, that the stockpiled chemical weapons of the world must be destroyed. This objective should also include the destruction of the thousands, if not millions, of unexploded chemical munitions which lie buried in the earth or sunk beneath the sea at uncertain locations. Those munitions, which can date from the war of 1914–18, are regularly unearthed by accident, or brought to the surface in the nets of fishermen or to our beaches by tides. Those unexploded munitions which have been dumped close to human activities need to be monitored and eventually destroyed.

To achieve this splendid objective we must first, as chemists, turn our attention to the various technical aspects of the problem. For example, how does one safely destroy thousands of tons of stockpiled chemical weapons? Or, how does one set about the destruction of a rusty old shell, of uncertain contents dug up on an old battlefield, and how can one destroy chemical weapons, of whatever type, without enormous expenditure that may be beyond the capacity of some nations?

Many chemists and engineers have worked on these problems and much has been learned of the relevant properties and chemistry of chemical warfare agents. Indeed, some good technologies for destruction of chemical munitions and agents have been developed.

The problem in hand – how best to destroy such materials? (Crown Copyright, printed with permission of the Controller, Her Majesty's Stationary Office.)

Nevertheless, progress in the destruction of chemical weapons has been slow, in part due to a paucity of scientific information on their chemical and physical properties, and because of the fierce opposition of ordinary citizens to certain technologies and, in particular, to the siting of these technologies near their homes.

To date, only small fractions of the stockpiles of chemical weapons agents of Russia and the United States, which are of order 30 000 tons each, have been destroyed despite government decisions having been taken to destroy them. In contrast, substantial quantities of chemical weapons which were in the possession of Iraq were destroyed by a United Nations team after the recent Gulf War. The team which destroyed the Iraqi weapons was, however, free of many of the constraints that restrict, and often retard, destruction work in other countries.

Valuable studies of current technologies for the destruction of chemical munitions, notably by committees of the US National Research Council and with particular reference to the US, have been made and published. Such studies have focused attention on the numerous gaps in our knowledge of the behaviour of these materials. Chemical defence scientists have identified other lacunae in informal conversations, but there has been little formal attention to these problems when this topic is viewed from an international perspective.

The IUPAC Task Force on Scientific Aspects of the Destruction of Chemical Warfare Agents, which is studying the general problem, met in Rome, Italy, 6–9 September 1994. The Task Force now offers some recommendations, relating mostly to general problems, discussed and approved in that meeting. Those problems and recommendations are presented here in abbreviated form.

A. Problems of Science and Technology

What is the fate of Chemical weapons Agents released into the environment?

Communities in the vicinity of sites where chemical weapons agents are stored, or where their destruction is planned, are naturally concerned that their immediate and long-term health should not be jeopardized by minor releases of chemical weapons agents that might occur due to accident or incompleteness of destruction. It might be expected from observation and from experience that small amounts of these agents released into the environment would be rapidly degraded by natural processes. There is however, a paucity of knowledge of actual degradation rates, of what products of degradation are formed, and what toxicity, if any, those products may have. Conceivable natural degradation processes include hydrolysis, photolysis by the action of sunlight, oxidation through the action of ozone and hydroxyl radicals in the atmosphere on sunny days, and biodegradation by soil bacteria and fungi. However, we known little about the efficiencies and mechanisms of these processes.

It is therefore imperative that some experiments be undertaken to obtain some answers to these questions of the possible degradation rates of chemical weapons agents in the environment.

The problem of recovered old munitions: what are they and what do they contain?

Many old chemical munitions, some dating from World War I, and many from World War II, still lie buried in the ground or sunk under water. They are occasionally recovered from old battlefields, or from old military posts, or from harbours or lakes, even in countries that did not themselves produce or possess chemical weapons agents. As found, these old munitions are usually highly corroded and one is uncertain as to their origin and/or their contents.

Does a recovered munition contain high explosive or various chemical agents? If the latter, which chemical weapons agent does it contain? It is desirable that one be able to answer these questions without opening the munition. There are methods for gaining answers to these questions, but they are often slow and the answers not fully satisfactory.

More effort should be put into discovering and developing superior methods for non-intrusive identification of the contents of recovered old munitions. Such technology would, of course, have very wide applications in many fields of analytical science.

The problem of gelled or crusty materials in containers of 'mustard'

HD (Mustard) is one of the oldest chemical weapons agents. It was used extensively in World War I and is a major item in stockpiles of chemical weapons agents manufactured subsequently. In HD munitions long buried in the ground or sunk at sea, and in tanks that have held HD in storage for decades, the HD has become partly or even mostly gelled or crusty. Such old containers often contain other hazardous gases, including hydrogen, that escape when the container is punctured or opened.

The gelled or solidified HD does not easily drain from opened containers. When the fluid portion has drained away, the remaining gels or crust often remain wet with HD. This is a hazard to workers and requires additional treatment to free the containers of HD before their disposal as scrap metal. To date, only incineration is an effective means of removing the residues. Conceivable use of chemical reactions to eradicate them is complicated by current ignorance of the chemical structure of the gelled or crusty material. Consequently, the chemistry of gelled or crusty HD (Mustard) should be thoroughly studied.

Prof. Joe Bunnett of the University of California, Santa Cruz, Chairman of the Task Force on Scientific Aspects of the Destruction of Chemical Warfare Agents.

The problem of ascertaining how much chemical warfare agent may remain after having been subjected to a destruction process

Knowing how completely a chemical weapons agent is destroyed by a particular destruction process is important. One must therefore perform chemical analysis of the products. The analysis should enable both detection and quantitative determination of the agent, accurately even at extremely low concentration levels. Although methods that probably meet this standard are known, it is not clear that the standard is met for all the major chemical weapons agents and all the chemical situations where these agents might exist.

Research to discover and develop superior analytical methods for detection and quantitative determination of any chemical weapons agent surviving destruction processes should be undertaken. Perhaps even developing new analytical techniques to identify all possible products.

Inadequacy of knowledge about the fundamental chemistry of chemical warfare agents

Since 1915, chemists have studied the chemistry and physical properties of numerous chemical weapons agents. However, many studies were made before powerful modern experimental techniques become available. Chemists working on the destruction of chemical weapons agents are often frustrated by gaps in fundamental knowledge of agent chemistry and physical properties. Knowledge of the chemistry of the arsenical agents needs especially to be expanded.

Rigorous research for systematic expansion of knowledge of the fundamental chemistry of chemical warfare agents, as relevant to their destruction, should be conducted.

Monitoring of air spaces and gas streams during storage and destruction of chemical warfare agents

The highest priority in storage and destruction of chemical weapons agents is the protection of humans from exposure. In view of the constant possibility of a leakage or of a spill of an agent, or that a destruction operation will be incomplete, it is desirable to have means for the immediate detection, even at the trace level, of any escape of chemical weapons agent within buildings used for storage or destruction. Several detection systems have been developed, but they are less than ideal. What is needed is a superior continuous, real-time monitoring system able to detect chemical weapons agents in the gas phase at very low concentrations, determining both the presence and the specific identity of the detected agent with rare false alarms.

Development of sensitive definitive methods and equipment for rapid monitoring of air spaces and gas streams should be undertaken. Again, this research would have many applications in fields far removed from the destruction of chemical weapons agents.

The problem of disposal of neutralization or scrubber brines

For the destruction of these agents, two prominent technological alternatives exist, incineration and neutralization with sodium hydroxide, both generate, in different ways, brines that contain sodium chloride and other salts dissolved in water. Many of those salts are normal constituents of sea salt. It is therefore conceivable that, if a chemical weapons agent destruction plant were constructed near the ocean, discharge of those brines directly into the ocean would not abuse the environment or harm marine life. A difficulty however, is that the brines often contain small amounts of salts of lead, mercury and other heavy metals. Before such brines could responsibly be discharged into the sea, methods to remove the heavy metal constituents would need to be developed. Possible environmental impacts would need to be evaluated by oceanographers.

Scientific questions regarding possible ocean discharge of brines resulting from destruction of chemical warfare agents should be investigated.

The possibility of combining destruction of a chemical warfare agent by neutralization with follow-up degradation of the intermediate products by wet air oxidation

Laboratory studies have indicated that several chemical weapons agents are destroyed by reaction with aqueous sodium hydroxide, yielding products of greatly reduced toxicity. In many cases the products formed must however, be further degraded, for safety and to meet legal requirements. It has generally been assumed that neutralization and follow-up degradation would be conducted as consecutive, but separate processes. Conceptually, it seems possible that neutralization and follow-up degradation by wet air oxidation could be combined into a single process. Wet air oxidation is a general term for oxidation by, for example, air, pure oxygen or hydrogen peroxide, of organic contaminates at low concentrations in water at temperature

around 250–300 °C. However, water at such high temperatures develops high pressure, which must be contained. To minimize corrosion, wet air oxidation is preferably conducted on alkaline solutions.

The feasibility of combining sodium hydroxide neutralization with wet air oxidation into an integrated process should be studied, with special attention to engineering considerations.

B. Problems of Information and Communication

As in many branches of science, there is a wide gulf between the scientist and the general public who support, with their taxes, the work of the scientist. Many, such ordinary people are completely disillusioned by science. Consequently, there is a particular problem with a subject as emotive as chemical weapons research, even if the end result is their destruction. Nobody will want this research in their back-yard.

The lay public is not adequately informed about technological aspects of the destruction of chemical weapons, and chemists should be urged to communicate with their fellow citizens by writing articles in language intelligible to layman, by giving public talks, and by participating in radio and television broadcasts.

The problem of communication also lies at the heart of the study of the properties and chemistry of the chemical weapons agents. Many studies were undertaken, however, they were undertaken by the military establishments of the different nations who built up these poisonous arsenals and, unfortunately, this information which was a militarily secret during the Cold War has not been made available to the public.

The chemists who did those studies or department heads who received their reports should make them available to all scientists of the world in one of three ways: preferably, by publication in peer-reviewed scientific journals; alternatively, as publicly available reports; or, for minor studies of good quality, by submission to the Technical Secretariat of the Organization for the Prohibition of Chemical Weapons, for inclusion in a data bank.

Although reports of much useful chemical weapons agent research are still kept secret, a great deal of such research is now available. However, it is often in government agency reports that are not abstracted by *Chemical Abstracts*. As a result many of those reports are extremely difficult for a chemist to locate, making them effectively unavailable.

A comprehensive bibliography of published or publicly available reports concerning properties and chemical behaviour of chemical weapons agents relevant to their destruction, to be available to all persons in all countries on payment of a modest charge, should be prepared.

This problem of carefully monitoring the destruction of chemical warfare agents has been highlighted by a recent explosion at the US Army's incineration facility on Johnson Atoll in the Pacific Ocean. On 19 November 1994, the 436th nerve-gas rocket to be decommissioned that day had just been emptied of its nerve-gas payload (nerve-gas agent GB) when it exploded. This was the first such explosion of a nerve-gas rocket being decommissioned and the force of the blast was contained with no nerve-gas contamination being detected.

The Army scientists are pleased with their safety record. So far, 37 000 rockets, mostly filled with nerve agent VX have been destroyed at the Johnson facility without incident. All nerve agents at the Johnson facility are delivered by a fluid injection system to the facility's liquid incinerator (*Chem. Eng. News*, 12 December, p. 27 (1994)).

The Task Force meeting to consider its recommendations.

New Directions for the *Chemical Abstracts*

The Chemical Abstract Service (CAS) of the American Chemical Society (ACS) is one of the world's oldest and greatest sources of chemical information. It has recently been put under new management and energized by a new innovative management team, who are adopting a more business-like approach where the abstract service now gives top priority to its customers.

In early November, the information world was given a preview of the new on-line information retrieval system of the CAS, SciFinder. This is not simply a new software package for finding information, but reflects the new attitude and substantial change that has been going on within the largest division of the ACS. SciFinder is the first intuitive, menu-driven information retrieval product of its kind in chemistry.

The CAS started as essentially a one man show in 1907, and was turned into a division of ACS in 1956. A pioneer in the computerization of scientific information, CAS developed the CAS Chemical Registry System in 1965 to identify and record chemical substances reported in the literature. In 1983, CAS created with Fachinformationzentrum (FIZ), Karlsruhe, Germany, a new on-line service called STN International. In 1987 the Japanese Information Centre of Science & Technology joined CAS and FIZ. Today, more than 188 scientific and technical databases are accessible through this network.

The best known of the CAS printed publications is *Chemical Abstracts* (CA). Each weekly issue contains more that 9500 abstracts of findings in chemistry, chemical engineering and related fields reported in journals, dissertations, conference proceedings, technical reports and books from around the world. In 1993, CAS offered the 12th Collective Index and a companion abstract product on CD-ROM. Since 1907, CAS has published more than 14 million abstracts of the chemical literature. Today, most of this information is available in print and via on-line databases.

Each year, CAS's scientists analyse, extract and index about 9000 scientific journals to select the information that will be summarized and included in its various information products. Projected production for 1994 is 640 000 abstracts, up 16% on 1993.

CAS currently has eight databases; CA (a bibliographic file providing access to information which has appeared in CA since 1967), REGISTRY (a companion file for chemical substance searching and identification. The largest file of substance information in the world. It may be searched by using structures, substances or text terms, including molecular formulae and chemical names. Proteins and nucleic acid sequences are accessible by inputting the desired string of amino acids or nucleotide codes.), CAOLD (access to data which appeared in CA before 1967), CAPreviews (gives a preview of documents which will appear in CA), CIN (an on-line version of the printed publication), CHEMLIST (contains information about chemicals subject to regu-

CAS staffer adds information to databases housed in state-of-the-art computers.

Located on a 55-acre campus near Ohio State University, Columbus, CAS's goal is to remain the world's leading provider of chemical information.

lation by the Environmental Protection Agency under the Toxic Substances Control Act), CASREACT (a file of more than 1 million organic chemical reactions appearing in the literature since 1985), and MARPAT (a file of Markush structures – generic chemical structures used legally to protect classes of compounds that have appeared in the patent literature since 1988). All are available on STN International.

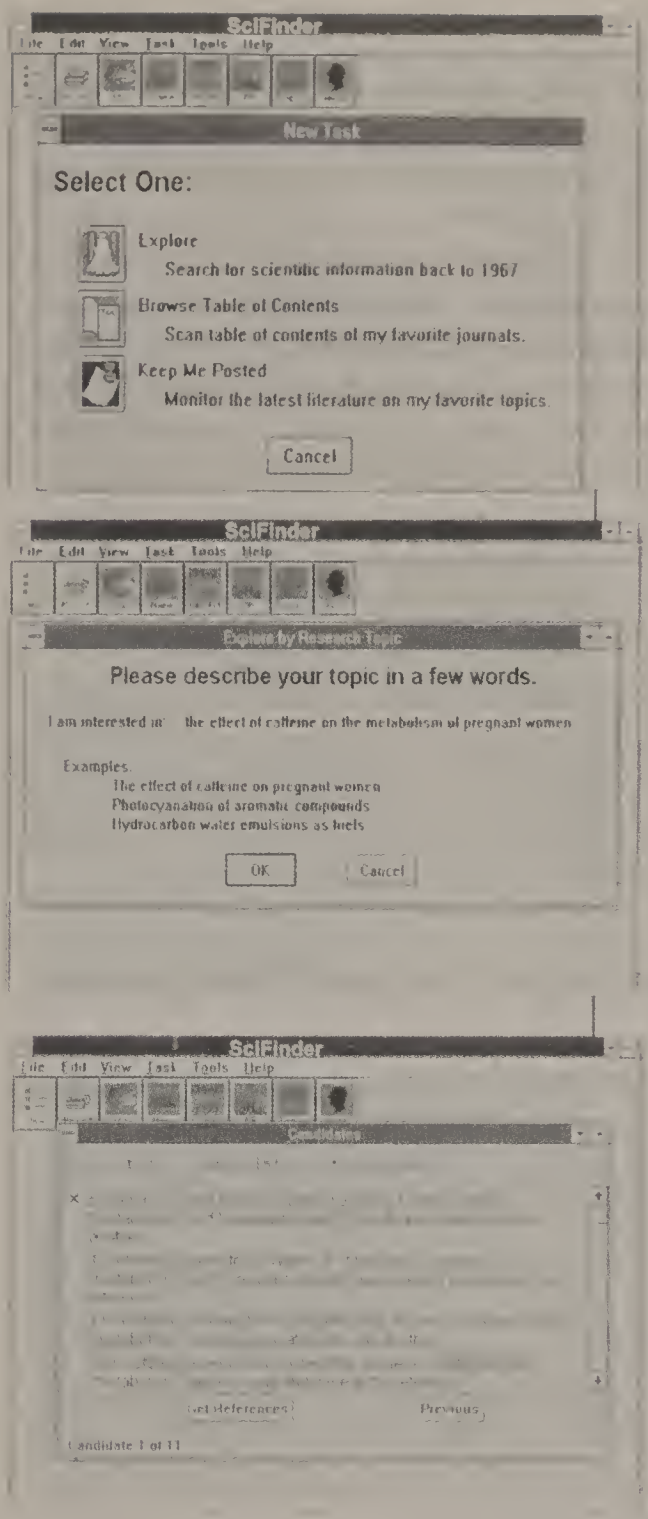
The CAS has always had a large market share of the on-line data retrieval business, however, it has been viewed with misgivings by some of its customers. In the past many customers used CAS because they had to use CAS; now with the approach of the new management team, people are using CAS because they want to use CAS. Robert J. Massie was appointed director of the CAS Division in mid-1992 and his goal is to turn CAS into the world's leading provider of chemical information. To achieve this goal, much effort has been devoted into running the division less like an institute and more like a focused customer-oriented information business which will win going into the 21st century.

The *Chemical Abstracts* on-line service grew up in the 1980s, it was an expert system which was sophisticated for the time, but required training to use. The new SciFinder system was introduced to the public in San Francisco in early November 1994 at Online/CD-ROM '94, an information industry trade show. The product is in the last phase of testing and is to go on sale in early 1995.

Linked to the CAS registry of more than 13 million substances and CAS databases with references to more than 11 million articles and patents, SciFinder will supply users with information ranging from chemical structures to chemical-related literature at their desk. The software system is immediately usable and user friendly without requiring special training. A user can look up an author, explore a research topic, find references to substances and preparative routes while also being able to browse through recent journal articles. It provides three pathways to CAS data, designated 'explore', 'browse table of contents', and 'keep me posted'.

For example, suppose a scientist had heard of a presentation on a specific subject and wanted to check CAS databases for other articles by the author. The only available information was the authors name, If the searcher had only a slight idea of the spelling of that name, most search software would register zero finds. A most dispiriting situation when using on-line searching techniques. SciFinder automatically comes up with several alternative spellings and gives a list of possible authors. SciFinder anticipates questions in ways that non-intuitive software cannot. It was designed so as to give the user a zero response as infrequently as possible.

Targeted users include chemists and similar researchers in petroleum, agriculture, consumer products, pharmaceutical, and biotechnology industries. SciFinder will work on Macintosh or Windows-based personnel computer systems.


SciFinder
New Task
Select One:
Explore
Search for scientific information back to 1967
Browse Table of Contents
Scan table of contents of my favorite journals.
Keep Me Posted
Monitor the latest literature on my favorite topics.
Cancel
SciFinder
Please describe your topic in a few words.
I am interested in: the effect of caffeine on the metabolism of pregnant women
Examples:
The effect of caffeine on pregnant women
Photocyanation of aromatic compounds
Hydrocarbon water emulsions as fuels
OK
Cancel
SciFinder

Screen output from CAS's SciFinder.

The Director is bullish in his view of the future, he wishes to ensure that CA is as accessible to individual scientists as evolving technologies permit. Put simply, a chemist in 1965 did not need any special training to go into the library and to understand the use of the printed version of Chemical Abstracts, we need an electronic product which is equally as straightforward to use. SciFinder fulfils this need, you just turn it on and search.

STN international has recently (November 1994) announced several new database facilities involving Japanese and American Patents.

The JAPIO database contains information relating to Japanese patent applications and is now available for public access. The JAPIO database offers the most comprehensive English language access to approximately 4.5 million Japanese unexamined patent applications (Kokai Tokyo Koho), covering all mechanical,

electrical, chemical, and physical technologies.

The USPATFULL database encompasses full texts of patents from the US Patent and Trademark Office since 1974, with limited coverage between 1971 and 1973.

These new additions complement the already existing STN product range. Besides JAPIO and USPATFULL, specific databases offer access to world-wide patent publications. For example, German patent information can be found in the well-known patent databases of the German Patent Office (PATDPA, PATGRAPH, PATD) as well as the PATOS files produced by the Wila-Verlag, containing patent publications of the German and European Patent Offices, and the World Intellectual Property Organization.

For further information, please contact: STN International, c/o FIZ Harlsruhe, PO Box 2465, D-76012 Karlsruhe, Germany. Tel. +49 7247 808 555. Fax +49 7247 808 259. Electronic mailbox STNmail: HLPDESKS; Internet hlpdeskk@fizkarlsruhe.de

Nominations for the Ewald Prize

The International Union of Crystallography is pleased to invite nominations for the Ewald Prize for outstanding contributions to the science of crystallography.

The prize is named after Prof. Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography (IUCr). Prof. Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first editor of the IUCr publication *Acta Crystallographica* from 1948 to 1959 and President of the IUCr from 1960 to 1963.

The prize, which is awarded triennially at the International Congress of Crystallography, consists of a medal, a certificate and a financial award. The prize has been awarded three times; to Prof. J.M. Cowley and Dr A. F. Moodie, Prof. Vainshtein and to Prof. N. Kato. The fourth prize, for which nominations are currently being invited, will be presented at the XVII Congress in Seattle, Washington, USA, in August 1996.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible for this prize, irrespective of age, experience or nationality. The selection committee will give careful consideration to the nomination of outstanding scientists who have not yet won a major prize.

Either an exceptionally distinguished scientific career or a major scientific accomplishment may be recognized. The prize may be shared by more than one contributor, but not more than three, to the same scientific achievement.

Nominations for the Ewald prize should be submitted in writing, preferably using the appropriate Ewald Prize Nomination Form and accompanied by supporting documentation, to the Executive Secretary of the International Union of Crystallography, 2 Abbey Square, Chester CH1 2HU, UK (Tel: +44 244345431, Fax +44 244344843, E-mail: execsec@iucr.ac.uk) from whom copies of the Nomination Form and the names of the Selection Committee may be obtained. The closing date for nominations is 31 August 1995.

Prizes for Promoting Science

Prof. John Emsley has won the inaugural Chemical Industries Association Presidents Award for his "outstanding contribution through the news media to the public understanding of science and public familiarity with the chemical industry".

The GBP10 000 award went to Prof. Emsley in recognition of his work on the Molecule of the Month feature, on caffeine, maleic anhydride, opium and phosphate amongst many other topics, in the newspaper *The Independent*.

His contributions to radio work were also being honoured by this prize, in particular, a piece on 'Mozart being poisoned by antimony not Salieri – how many symphonies did antimony write?'

The Council of the Royal Society has made the Michael Faraday Award for 1994 to Sir Walter Bodmer FRS, Director-General of the Imperial Cancer Research Fund, in recognition of his outstanding achievement in raising the public understanding of science and technology as an issue of the highest importance to individual scientists and engineers and to many of the bodies who represent them.

Sir Walter was a founder member of COPUS (Committee on the Public Understanding of Science). This committee has become the reference point and spur for many new initiatives, and has stimulated and assisted actions nation-wide.

Evidence for Element 110

A collaboration between the Gesellschaft für Schwerionenforschung (GSI) in Darmstadt, Germany, the Flerov Laboratory of Nuclear Reactions at Dubna, Russia, the Department of Nuclear Physics, Comenius University in Bratislava, Slovakia, and the Department of Physics of the University of Jyvaskyla in Finland have recently announced experimental evidence for the creation of element 110.

In an experiment to identify element 110, the scientists observed an alpha-decay chain that can be unambiguously assigned to the specific isotope of element 110, $^{269}110$. In a series of experiments, the excitation functions of the fusion reactions $^{50}Ti + {}^{208}Pb \rightarrow {}^{258}104^*$ (dubnium) and $^{58}Fe + {}^{208}Pb \rightarrow {}^{266}108^*$ (hahnium) were

measured with high precision in order to determine the optimum projectile energies for the production of these heavy elements. These experiments involve accelerating one of the atoms, which has been stripped of its electrons, and colliding this accelerated particle into an appropriate target. From a detailed study of the optimized experimental conditions necessary for the production of elements 104 and 108, for example, the acceleration conditions, it is possible to determine the optimum conditions for the production of the heavier elements. The cross-section maxima of the neutron evaporation channels were observed at excitation energies of 15.6 MeV and 13.4 MeV, respectively. It was found that these data result in an optimum excitation energy for 12.3 MeV of the compound nucleus for the production of $^{269}110$ in the reaction $^{62}Ni + ^{208}Pb \rightarrow ^{269}110$ + neutron.

The idea is to produce the new nucleus with as little excitation as possible – cold fusion. This occurs when the projectile ion is given just enough energy, electrostatic acceleration of the ion in an applied laboratory field, to overcome the electrostatic repulsion of the target nucleus, producing a super-heavy nucleus with little residual energy.

Further observations showed a subsequent decay chain of three consecutive alpha-decays. Thus, it is reasonable that the originally formed compound nucleus could be assigned to the isotope with a mass number 269 of the element 110 (on the basis of alpha-decay coincidences). The accurately measured decay data of the daughter isotopes of the elements 108–102 obtained in previous experiments were used in the data analysis. The isotope $^{269}110$ is seen to decay with a half-life of 270 microseconds by emission of 11.132 MeV alpha-particles.

The new element is not created very rapidly. After the cooled target had been exposed to a million million accelerated ions per second, the team identified an atom of 110 in 2 days of bombardment. Most of the accelerated ions pass straight through the target. However, the group had anticipated that it might have taken them 2 weeks to produce one atom.

The decay chain may be written:

$^{62}Ni + ^{208}Pb \rightarrow ^{269}110$ (unstable compound nucleus)
$\rightarrow ^{265}108$(hahnium) + alpha-particle
$\rightarrow ^{261}106$(rutherfordium)+ alpha-particle
$\rightarrow ^{257}104$(dubnium) + alpha-particle.

For the moment, researchers are waiting anxiously to see if other laboratories will be able to duplicate these experiments at GSI. A joint US–Russian team working at Dubna, Russia, began an experiment to produce element 110 two months before the German group, but they have only just began to analyse their data. Likewise, earlier this year, a team at the Lawrence Berkeley Laboratory, USA, re-analysed some data from experiments on heavy element production performed in 1991 and may have some evidence for the creation of element 110.

The Russian experiment at Dubna is very different in that they use hot fusion where plutonium nuclei are bombarded with sulfur ions with more than enough energy to fuse. Consequently, the product compound nucleus cools off by evaporating neutrons. If the Russian experiment works, the nuclei of their isotope of element 110 will have 163 neutrons, compared to the 159 and 161 produced by GSI.

Although the paper describing these exciting new results will be published quite soon, probably before we go to press, in *Zeitschrift für Physik*, the scientists involved in these experiments are refusing to suggest a name for the new element. Indeed, their reticence is strongly linked to the continued furore over IUPAC's recommendations for the names of elements 100–109.

As reported in the previous issue of *Chemistry International* and in this issue, the long-standing controversy over the names of the transfermium elements was resolved in September 1994 when the IUPAC Commission on Inorganic Nomenclature issued its recommendations for the names for the most recently discovered heavy elements. However, the IUPAC choice of names has angered many scientists who work in this field.

Many physical chemists were unhappy that the name rutherfordium (after Ernest Rutherford) had been given to element 106. This name had previously been tentatively assigned to element 104, indeed, this tentative assignment had been 'in the literature' for more than twenty years. The name suggested by the Californian laboratory which discovered element 106 was seaborgium after the Nobel Laureate Glenn T. Seaborg. However, the IUPAC Commission felt it inappropriate to name an element after a living person. As there could, in this way, be no historical perspective given to the work.

The German laboratory who have now found element 110 have been caught up in this controversy because they identified elements 107, 108 and 109 and had consequently suggested names for their discoveries.

The German discoverers are, however, unhappy about the names finally suggested by the IUPAC Commission. The Germans had originally suggested neilsbohrium (107) after Niels Bohr, hassium (108) after the Latin name for the region of Germany where their laboratory is situated (Hesse), and meitnerium (109) after the Austrian scientist Lise Meitner. But the names suggested by IUPAC are bohrium, hahnium and meitnerium, respectively. Unfortunately, the name hahnium, after the German scientist Otto Hahn, had previously been tentatively assigned to element 105 after its discovery in 1970.

The senior scientists at the GSI are irritated that their choices for names, which as Peter Armbruster the Di-

rector says are the prerogative of the discoverers, have been ignored or changed by the Commission on Inorganic Nomenclature. They feel that if the Commission did not wish to use their original suggestions, then they should have told them so that they could have come up with other names.

At the moment there is confusion on this subject. The final decision on the IUPAC recommendation for the names of these elements will be taken at the General Assembly in Guildford next August and until then there are two sets of nomenclature for these heavy elements.

Element	IUPAC recommended name	Other name
104	dubnium	rutherfordium
105	joliotium	hahnium
106	rutherfordium	seaborgium
107	bohrium	nielsbohrium
108	hahnium	hassium
109	meitnerium	meitnerium

Such disagreements over the name of a chemical element are unfortunately not new. In 1950, IUPAC had to intervene after almost a century of controversy to recommend that the name of element number 41 be niobium. As one of the first specimens of the ore containing this element was found early in the 18th century in the North American Colonies (by John Winthrop the first Governor of Connecticut, but send to England for study) many American chemists and institutions continued, after it's isolation in 1864, to refer to this element as columbium (Cb). Indeed, this non-IUPAC-recommended name may still be seen in some metallurgical industry literature from the US.

Correction

Naming of the Transfermium elements (Chem. Intl. **17** (1), 3–5, 1995). In this comment on the origin of the names of the transfermium elements, it was implied that nobelium (No), element 102, was discovered by the Berkeley group in 1958. This, however, is something of an oversimplification in that many groups had published observations on this element subsequent to 1957 (Stockholm–Harwell–Argonne, 1957; Dubna, 1958, 1958, 1960, 1963, 1964, 1965, 1966; Berkeley, 1958, 1959, 1961, 1967; Stockholm–Argonne, 1959; and Oak Ridge, 1971). However, the Transfermium Working Group (TWG) of IUPAC and IUPAP (created to set-up discovery profiles for the transfermium elements), after considering the literature and the various technical difficulties of the different measurements, decided (*Pure Appl. Chem.* **65**, 1757–1814, 1993), 'The two 1966 (simultaneously published) Dubna results, both submitted in 1965, give conclusive evidence that 102 has been produced.'

Names and addresses

Full details (names, addresses, telephone/telex/fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* **15**, 215–227 (1993). The IUPAC Secretariat have been notified of the following changes:

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Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chem. Intl.* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most up-to-data list of the national/regional centres appeared in *Chem. Intl.* **14**, 25 (1992) and in the latest *IUPAC Handbook* (1994–1995) published by Blackwell Science, 1994.

Non-Linear Macromolecules

The document, *Source-Based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies*, has been prepared by a working party of Commission IV.I to begin its public review process.

The recommendations for macromolecular nomenclature published to date have dealt only with: regular single-strand organic macromolecules, regular single-strand and quasi-single-strand inorganic co-ordination macromolecules, and copolymer macromolecules. As far as it is possible, the established principles of organic and inorganic nomenclature have been followed.

The present document, is intended to extend the system of nomenclature to nonlinear macromolecules such as branched and cyclic macromolecules, micronetworks, polymer networks, and to macromolecular assemblies which are held together by weak, van der Waals or non-covalent bonds, such as polymer blends, interpenetrating polymer networks, and polymer complexes.

To begin with, the word 'polymer' is itself somewhat ambiguous. It is commonly used to refer both to polymer substances and polymer molecules, that is, to the polymerized monomer and to the monomer itself. The present document is concerned solely with the nomenclature of molecular structures, 'macromolecule' is used for individual monomer molecules and 'polymer' is used to denote a substance composed of macromolecules. Both 'polymer' and 'macromolecule' are used as adjectives according to accepted usage, for example, 'polymer blend' and not 'macromolecular blend'.

For nonlinear macromolecules, the skeletal structure should be reflected in the name and nonlinear macromolecular structures and macromolecular assemblies are classified using the following terms:

- Cyclic;
- Branched, short- and long-branched;
- Micronetwork;
- Network;
- Blend;
- Semi-interpenetrating polymer network;
- Interpenetrating polymer network;
- Polymer-polymer complex.

The names of nonlinear macromolecules are formed by citing the source-based name(s) of the constituent linear chain(s) and denoting their mode (s) of combination by prefixes and connectives. Specification of molecular weight, composition or branch-point functionality(ies) of the macromolecule or of its constituents may be given in parentheses.

Some examples: a sample of polystyrene cross-linked with a small quantity of divinylbenzene, but not sufficient to form a network, would be designated branch-polystyrene-v-divinylbenzene, in the new nomenclature. A variegated star copolymer molecule consisting of arm(s) of polyA, arm(s) of polyB and arm(s) of polyC, would now be termed star-(polyA; polyB; polyC). An example of a complex of statistical copolymer and homopolymer molecules would be, poly[(methyl methacrylate)-stat-(methacrylic acid)]-compl-poly(N-vinyl-2-pyrrolidone).

Comments on these recommendations are welcome and should be sent by 1 August 1995 to:

Dr Jaroslav Kahovec, Institute for Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovskeho namesti 2, CS-162 06 Praha 6, Czech Republic.

Schematic representation of macromolecular assemblies which the present rules of nomenclature are attempting to rationalize.

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *PAC*.

Names and Symbols of Transfermium Elements (IUPAC Recommendations 1994)

Recommendations for the names and symbols of the transfermium elements (atomic numbers 101–109) are presented along with the reasons for proposing them.

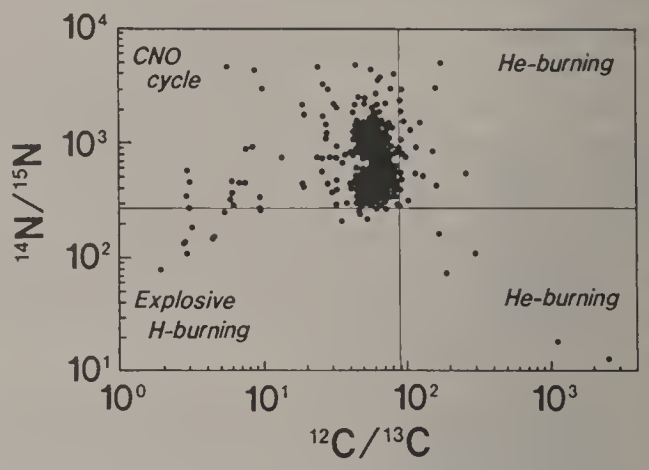
This IUPAC Recommendation has, since it was first made public, generated considerable controversy. See also the Secretary General's Column and News and Views section for further details.

The report was prepared for publication by the Commission on Nomenclature of Inorganic Chemistry of the Inorganic Chemistry Division. The Chairman of this Commission is Professor A.M. Sargeson of the Australian National University, Canberra, Australia. The full details are published in Pure Appl. Chem. ***66****, 2419–2421 (1994).*

Atomic Weights of the Elements 1993

The biennial review of atomic weight, A_r(E), determinations and other cognate data has resulted in changes for the standard atomic weight of titanium from 47.88 ± 0.03 to 47.867 ± 0.001, of iron from 55.847 ± 0.003 to 55.845 ± 0.002, of antimony from 121.757 ± 0.003 to 121.760 ± 0.001, and of iridium from 192.22 ± 0.03 to 192.217 ± 0.003. Recent investigations on chlorine and bromine confirmed the currently accepted values of A_r(Cl) and A_r(Br). To emphasize that the atomic weight of lithium commonly available in laboratory reagents can vary significantly, the value of A_r(Li) is footnoted.

As a result of several changes, the Tables of Standard Atomic Weights Abridges to Five Significant Figures has been updated. Because relative isotope ratio data for stable hydrogen, carbon and oxygen are commonly being expressed on non-corresponding scales, the Commission recommends that such isotope data be expressed only relative to the references VSMOW and VPDB. As many elements have a different isotopic composition in some non-terrestrial materials, recent data on non-terrestrial materials are included here for the interested scientific community.



The isotopic composition of nitrogen and carbon in interstellar SiC granins (average size 5 μm) separated from the carbonaceous chondrite Murchison. Variations over several order of magnitude are apparent. Most SiC granins fall into the quadrant corresponding to hydrostatic H-burning by the CNO-cycle. But a few grains are observed to fall in the other three quadrants, including that corresponding explosive H-burnings. Thus, these SiC grains are expected to have been produced from different stars and during various stages of nucleosynthesis.

This report was prepared by the members of the Commission on Atomic Weights and Isotopic Abundances of the Inorganic Chemistry Division. The details are published in Pure Appl. Chem. ***66****, 2423–2444 (1994).*

Formulae) of Macromolecules (IUPAC Recommendations 1994)

The unambiguous graphic representation of molecules is especially important for macromolecules, which often exhibit a larger number of structural features that do molecules of low molecular weight. For example, the formula of a copolymer should immediately imply if it is meant to represent a block copolymer or a copolymer with an unspecified sequence of monomeric units. Thus, a two-block copolymer consisting of a block containing p monomeric units A and a block comprising q monomeric units of B is represented by the formula $–(A)_p–(B)_q–$ whereas the corresponding random copolymer is represented by the formula $–(A–/–B)_n–$ where p + q = *n*.

This document provides rules and examples for the graphic representation of constitutional repeating units and monomeric units, regular and irregular polymers of simple as well as complex structures, including organic, inorganic homopolymers, alternating and periodic copolymers, statistical, random and unspecified co-

polymers, block copolymers and graft copolymers, including star polymers. The proposed graphic representations are suitable for implementation on graphic computer programmes.

This report was prepared for publication by a working group consisting of R. E. Bareiss (Germany), J. Kahovec (Czech Republic) and P. Kratochvil (Czech Republic). This working party is part of the Commission on Macromolecular Nomenclature of the Macromolecular Division. The details are published in Pure Appl. Chem. ***66**, 2469–2482 (1994).*

Terminology and Notations for Multistep Electrochemical Reaction Mechanisms (IUPAC Recommendations 1994)

Terminology and notation for a compact description of the mechanisms of electrochemical reactions occurring at and near an electrode during the passage of a current are given. These recommendations allow a detailed description of a sequence of chemical changes from a reactant to a particular product.

This report was prepared for publication by Claude P. Andrieux, Laboratoire d'Electrochimie Moléculaire, Université Paris, 2 place Jussieu, 75251 Paris Cedex 05, France, who is a Titular Member of the Commission on Electrochemistry of the Physical Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 2445–2450 (1994).*

Basic Classification and Definitions of Polymerization Reactions (IUPAC Recommendations 1994)

Polymerization reactions have traditionally been classified as addition polymerizations and condensation polymerizations. However, developments in chemical methods of polymerization and synthesis of new types of polymer have meant that more than two classes of polymerization need to be defined if a clear terminology is to be achieved. Several, alternative, two-fold terminologies have been introduced ad hoc into the literature. All have serious shortcomings in terms of comprehensiveness, ambiguity and scientific correctness.

This set of recommendations defines four basic categories of polymerization – chain polymerization, condensative chain polymerization, polycondensation and polyaddition – which cover unambiguously all presently known types of polymerization. The definitions also allow further qualification if desired, e.g. cationic chain polymerization.

The present recommendations are in accord with the recommended *IUPAC Glossary of Terms for Physical Organic Chemistry* (1983) and the *IUPAC Basic Definitions of Terms Relating to Polymers* (1974).

This report was prepared for publication by a working group consisting of I. Mita (Japan), R. F. T. Stepto (UK) and U. W. Suter (Switzerland). This working party is part of the Commission on Macromolecular Nomenclature of the Macromolecular Division. The details are published in Pure Appl. Chem. ***66**, 2483–2486 (1994).*

Nomenclature of Thermometric and Enthalpimetric Methods in Chemical Analysis (IUPAC Recommendations 1994)

This report defines the scope of enthalpimetric analysis within the general field of calorimetry and also delineates it as distinct from the general methods of thermal analysis for solid materials. Enthalpimetric analysis is also defined as a variant of calorimetry in which the enthalpy change of a chemical reaction is measured in order to perform a relatively rapid quantitative determination of an analyte, and in which at least one reactant is a liquid or a solution. Nomenclature is recommended for variations of the methodology in which the reaction is carried out as a titration, as a batch reaction, in flowing streams, or as an injection into flowing streams.

This report was prepared for publication by J. W. Stahl, Department of Chemistry, Geneva College, Beaver Falls, PA 15010, USA, who is an Associate Member of the Commission on General Aspects of Analytical Chemistry of the Analytical Chemistry Division. The report was prepared in conjunction with the Commission on Thermodynamics of the Physical Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 2487–2492 (1994).*

Classification and Definition of Analytical Methods Based on Flowing Media (IUPAC Recommendations 1994)

This report attempts to classify analytical methods based on flowing media and to define and standardize terminology. After classification and discussion of terms describing the systems and component parts, a section is devoted to terms describing the performance of flow systems. The list of terms included is restricted to those which are most relevant, in particular, self-explanatory terms are omitted.

Although belonging to the category of methods based on flowing media, chromatographic methods are not comprised in the present document. However, care has been taken to ensure that the present text is not in conflict with definitions used routinely in the domain of chromatography.

In documents in which flow methods are described, it should be clearly indicated how the sample and/or reagent is introduced and how the sample zone is transported. When introducing new techniques into the field, or new variants of existing techniques, it is strongly recommended that descriptive terms, perhaps based on the fluid dynamics, rather than trivial or elaborate names are used.

This report was prepared for publication by Willem E. van der Linden, Laboratory for Chemical Analysis, Department of Chemical Technology, University of Twente, PO Box 217, NL-7500 AE Enschede, The Netherlands, who is Secretary of the Commission on General Aspects of Analytical Chemistry of the Analytical Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 2493–2500 (1994).*

Nomenclature for Radioanalytical Chemistry (IUPAC Recommendations 1994)

Nearly 200 terms, commonly used in radioanalytical chemistry are unambiguously defined. The list is partially based on an earlier IUPAC glossary (*Pure Appl. Chem.* **54**, 1533–1554 (1982)), but some modifications have been made, terms relating to nuclear physics and technology have not been reconsidered and numerous new entries from the fields of radiometric analysis, radioimmunoassay and related topics have been included.

This report was prepared for publication by R. van Grieken, Department of Chemistry, University of Antwerp (UIA), B-2610 Antwerp-Wilrijk, Belgium, and M. de Bruin, Interfaculty Reactor Service, NL-2629 JB Delft, The Netherlands, who are members of the Commission on Analytical Nomenclature of the Analytical Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 2513–2526 (1994).*

Compilation and Critical Evaluation of Structure-Reactivity Parameters and Equations: Part 1 Values of σ_m and σ_p Based on the Ionization of substituted Benzoic Acids in Water at 25 °C (Technical Report)

Data have been compiled for the pK_a values in water at 25 °C of about 60 meta- and para-substituted benzoic acids, with a view to proposing recommended values of Hammett substituent constants, σ. Over 30 different substituents are considered, but for certain substituents data are not available for both the meta and the para position. The amount and the reliability of the data vary greatly from one acid to another. Critical appraisal of the available data leads to a classification of the substituents and their derived σ values as belonging to a first division (more reliable data) or a second division (less reliable data). The substituents in the former category are Me, NO_2, OMe, F, Cl and Br (each in both the meta and para position. Recommended values of σ are tabulated for substituents in each division, but for certain members of the second division there are caveats because the data show discrepancies.

Prepared for publication by John Shorter, School of Chemistry, University of Hull, Hull, North Humberside, HU6 7RX, UK, who is a Titular Member of the Commission on Physical Organic Chemistry (Working Party on Structure-Reactivity Parameters and Equations) of the Organic Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 2451–2468 (1994).*

Glossary of Bioanalytical Nomenclature Part 1: General Terminology, Body Fluids, Enzymology and Immunology (IUPAC Recommendations 1994)

Many disciplines are involved in the practice of clinical laboratory medicine, with each having its own set of technical terminology. Consequently, the terminology used in the clinical laboratory is often vague, inexact, and, in some cases, in discord with conventional and officially sanctioned terminology. In order to help rectify this situation, a general set of bioanalytical definitions has been compiled and collated from the documents of several national and international organizations, with the emphasis on those prepared by the International Union of Pure and Applied Chemistry and the International Union of Biochemistry.

References are included for each definition. This document contains sections on General Terminology, Body Fluids, Enzymology and Immunology. Other topics will be included in future documents. It is hoped that this set of bioanalytical definitions will be useful to the practitioners of clinical chemistry and will foster improved communication and understanding among them.

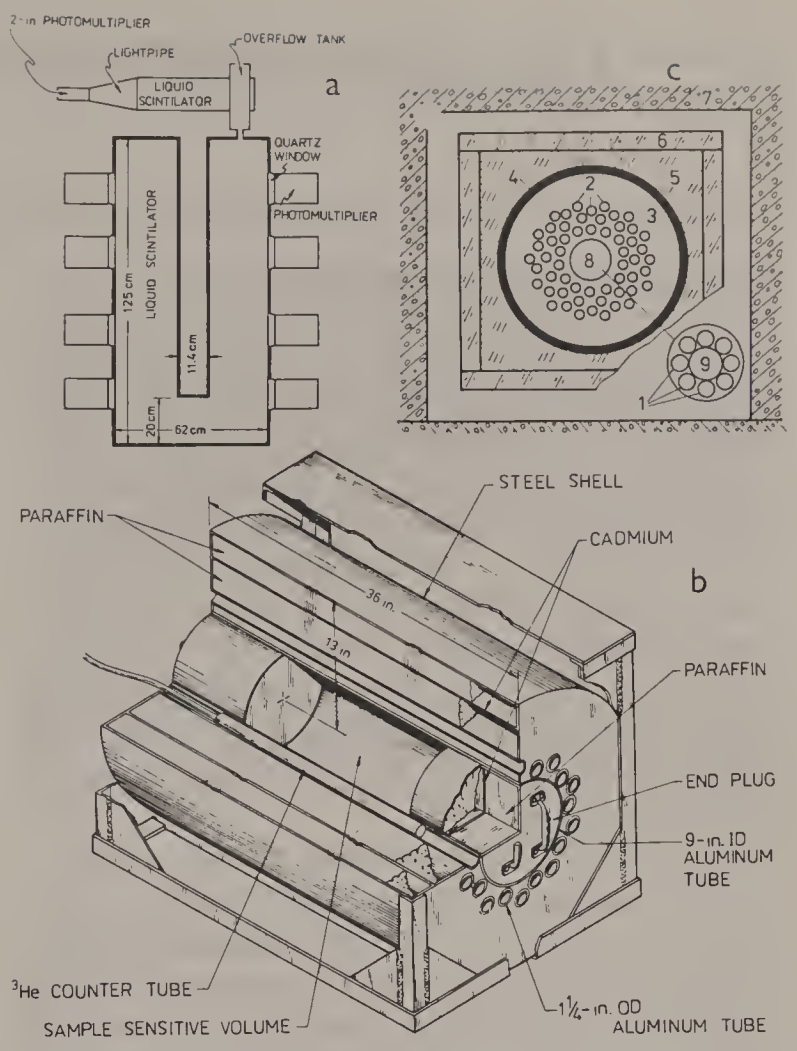
This report was prepared for publication by Carl A. Burtis, Clinical Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, and T.D. Geary, Institute of Medical and Veterinary Science, Frome Road, Adelaide, Australia, who are members of the Commission on Automation and Clinical Chemistry Techniques of the Clinical Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 2587–2604 (1994).*

Determination of Very Low Levels of Radioactivity (Technical Report)

This evaluation of different techniques, equipment and dedicated facilities for measurement of very low levels of radioactivity is intended for the large community of scientists who use radioactive tracers, who make activation analyses, or who may occasionally face the problem of measuring an activity well below the level accessible with standard commercial equipment. Emphasis is placed on the instrumental gamma-spectrometric assay of complex mixtures of radionucleotides, on the spectrometric measurements of alpha activities in relatively massive samples, and on counting spontaneous fission events in samples of large mass and/or volume.

A list of institutions and agencies which are active in developing low-level counting methods is given.

Prepared for publication by I. Zvara (Joint Institute for Nuclear Research, Dubna, Russia), P. Povinec and I. Sykora (Comenius University, Bratislava, Slovakia) who are Members of the Commission on Radiochemistry and Nuclear techniques of the Analytical Chemistry Division. This work benefited from a contribution by M. Sakanoue (Low Level Radioactivity Laboratory, Faculty of Science, Kanazawa University, 923-12 Japan). The details are published in Pure Appl. Chem. ***66**, 2537–2586 (1994).*



Neutron multiplicity counters. (a) Gd-loaded liquid scintillator at LBL, Berkeley; (b) moderator +^{3}He counters at ORNL, Oak Ridge; (c) moderator + ^{3}He counters + BGO trigger at JINR, Dubna; 1, BGO detectors; 2,^{3}HE counters; 3, moderator; 4, Cd; 5, polyethylene; 6, plastic scintillator; 7, concrete; 9, sensitive volume; 9, sample volume.

Factors Important in the selection and Description of Liquid–Liquid Extraction Procedures Used in Inorganic Analytical Chemistry (Technical Report)

This report deals with liquid–liquid distribution systems, in which one phase is aqueous and the distribution of the component can be influenced with chemical reactions. The formulae and equations are given, by which the actual distribution ratio of the analyte, at given conditions and concentrations, may be predicted. The conditional extraction constants, which are used in the calculation of the final distribution, may be calculated from the real extraction constants and side reaction functions involving the competing chemical reactions, and their equilibrium constants.

The kinetic aspects of the distribution process, the current analytical techniques, the analytical methods involving liquid–liquid distribution, the fields of application of liquid–liquid extraction are briefly introduced. A classification scheme of the extraction systems used in analytical chemistry is proposed in which the basic reaction equations are given, from which the extraction constant, the distribution ratio of the analyte can be formulated, and using the formulae, and the necessary equilibrium constants, the attainable extent of extraction (fraction extracted) may be estimated.

Prepared for publication by J. Inczédy, Veszprém University, H-8200 Veszprém, Hungary, who is a Member of the Commission on General Aspects of Analytical Chemistry of the Analytical Chemistry Division. The details are published in Pure Appl. Chem. ***66**, 2501–2512 (1994).*

Corrections to Recommendations

IUPAC–IUB Joint Commission on Biochemical Nomenclature Nomenclature and Symbolism for Amino Acids and Peptides (Corrections to Recommendations 1983)

Three corrections should be made in the document published in *Pure Appl. Chem.* **56**, 595–624 (1984).

The correct text may be found in *Eur. J. Biochem.* **213**, 1–3 (1993).

Publications

Advanced polymer materials

The May issue of *Die Makromolekulare Chemie: Macromolecular Symposium* (Vol. **83**, 1–323) sees publication of a collection, though incomplete, of the invited lectures delivered at the International Conference on Advanced Polymer Materials, which was held under the auspices of IUPAC in Dresden, in September 1993. Organized by the Institute of Polymer Research Dresden and the Dresden University of Technology, the conference sought to encourage scientists working in different fields of polymer research to discuss latest findings and prospectives in the development of new polymeric materials.

The conference brought together more than 200 scientists from academic and industrial research institutions in 24 countries from all over Europe and overseas. Some 80 papers and 70 posters were presented on the different topics. According to symposium chairman and editor, Hans-Jörg Jacobasch, the programme was well received and many participants emphasized the pleasant atmosphere of the meeting, which stimulated new contacts and discussions between the scientists. The meeting was held in six sessions: high performance polymers; surface and interface phenomena; reactive processing of polymers; characterization; structure/property relationships; cellulosics.

New CODATA Books

The Committee on data for Science and Technology (CODATA) was established in 1966 by the International Council of Scientific Unions. Working on an interdisciplinary basis, CODATA seeks to improve the quality, reliability, processing, management, and accessibility of data of importance to science and technology.

Activity Coefficients at Infinite Dilution, Vol. IX, Part 3. J. Gmehling, J. Menke and M. Schiller. DECHEMA Chemistry Data Series, Frankfurt, Germany (1994) 505 Pages. Price for parts 3 and 4 together DEM 690. ISBN: 3926959 46 0.

Activity Coefficients at Infinite Dilution, C_{10} – C_{36} with SO_2 and H_2O – Supplement, Vol. IX, Part 4. J. Gmehling, J. Menke and M. Schiller. DECHEMA Chemistry Data Series, Frankfurt, Germany (1994) 568 Pages. Price for parts 3 and 4 together DEM 690. ISBN: 3926959 47 9.

Manual on the Building of Materials Databases. Eds C. H. Newton. ASTM, 1916 Race Street, Philadelphia, PA 19103–1187, USA (1993) 105 pages, USD45.

ASTM Standards on the Building of Materials Databases. ASTM, 1916 Race Street, Philadelphia, PA 19103-1187, USA (1993) 112 pages, USD43.

Guide to Database Distribution. J. Bremmer. NFAIS, 1518 Walnut Street, Suite 307, Philadelphia, PA 19102, USA (1994) USD175.

AOAC International

AOAC International (formerly the Association Official Analytical Chemists) is a professional scientific association whose primary purpose is to promote chemical and biological methods validation and quality measurements in analytical chemistry. In addition, AOAC International produces a number of publications; in particular, they will release the 16th edition of the official *Methods of AOAC International* in January 1995. This substantial publication provides over 2100 chemical and biological methods for food, pharmaceutical, agricultural, environmental and other analysis.

Each AOAC Official method included in the Official Methods has undergone detailed laboratory collaborative testing and validation to ensure reliability of the method, and precision and accuracy of the data generated by the method.

This latest edition contains 149 new and 103 revised methods, a more accessible format and a more comprehensive index.

The new methodology and applications in the 16th edition include: enzyme-linked immunoassay techniques in nearly every analytic field, chemical methods for microbiological assays, methods for *Salmonella*, *Listeria*, *Vibrio*, *E. coli* and other coliforms, methods for water and soil contaminants, liquid chromatography methods for toxin analysis, hard surface carrier testing for disinfectant efficacy, and combustion methods.

The purchase price for the two-volume set is USD359 in North America (USA, Canada and Mexico) and USD399 outside North America. For more information, or to order a copy, please contact:

AOAC International, 2200 Wilson Blvd., Suite 400, Arlington, VA 22201–3301, USA, Tel: +1703 5223032

Change of British Telephone Numbers

OFTEL, the telecommunications regulatory body for the United Kingdom, has announced that 16 April 1995 will be Phoneday. By this date everyone in the UK will have a new telephone and Fax number.

At 1.00 am on Sunday 16 April 1995 the British area dialling codes will change.

When dialling from abroad, an additional digit 1 must prefix the local area code. Area codes starting 0 will start 01. For example, when dialling from outside the UK, the telephone number of the Oxford secretariat is currently, +44 865747744, after 16 April 1995 it will become, +44 1865747744. Likewise, our Fax number will become, +44 1865747510. The E-mail address will be unchanged.

Although these changes will become established after 16 April, the new area codes are working at present.

Translation of IUPAC Publications

A Polish translation of *A Guide to IUPAC Nomenclature of Organic Compounds* has recently appeared (Przewodnik do nomenklatury zwiazków organicznych).

The translation and the preparation of the manuscript was undertaken by Dr Barbara Szechner, Pharmaceutical Research Institute, Warsaw, Poland).

This translation is available from Professor Osman Achmatowicz, The Polish Chemical Society, ul. Freta 16, 00-227 Warsaw, Poland.

Of the same text, there now exists a translation into French, *Nomenclature UICPA des Composés Organiques*.

This translation has been prepared by Robert Panico (Professeur honoraire, École supérieure de physique et chimie industrielles) and Jean-Claude Richter (Professeur titulaire, Université de Montréal) and is published by; Masson Éditeur, 120 boulevard Saint-Germain, 75280 Paris Cedex 06, France, Tel: +33 1 40 46 60 00 (1994 ISBN: 2-225-84479-8).

Also recently available are translations into Hungarian of: *Names for Hydrogen Atoms, Ions and Groups, and for Reactions Involving Them* and the *Nomenclature of Hydrides of Nitrogen and Derived Cations, Anions and Ligands* (*A hidrogénatomok, -ionok és -csoportok, valamint a velük kapcsolatos reakciók neve* and *A nitrogén-hidrideknek, származtatott kationjaiknak, anionjaiknak és ligandumaiknak a nevezéktana*).

These translations are available from Dr Piroska Fodor-Csányi, Naphegy tér 5/b, H-1016 Budapest I, Hungary (Tel: +36 11755 732).

CHEMRAWN

A meeting of the CHEMRAWN Committee took place in Seoul, Korea, on 5–6 May 1994. Topics discussed included:

CHEMRAWN VII

The recommendations from the meeting are being distributed by American Chemical Society. These proceedings were published in book form by Blackwell in March 1994 with the royalties being used to help finance the follow-up programme. Of particular interest was one project relating to atmospheric studies in South America.

One of the current great mysteries concerning the chemistry of the atmosphere is the carbon imbalance. Our understanding of the production and loss of carbon, mostly in the form of CO_2, into and from the atmosphere is out-of-balance by 30–40% – where are the sinks for this CO_2? There is a serious lack of information on the carbon balance in a number of locations, including the Amazon, Central Africa and South-East Asia.

CHEMRAWN Committee during their meeting in Seoul, Korea.

The programme suggested at the CHEMRAWN meeting was to measure the concentrations, at 5–6 km altitude with inexpensive kites, of ozone, CO_2, CFC and other 'greenhouse' gases in the Amazon Basin. This programme would be undertaken jointly with DuPont-Brazil, the Universities of Sao Paulo, Brazil, Colorado, USA, and NOAA.

This project has been partially financed, however, more money will be needed to complete the study. the CHEMRAWN Committee does not have a direct responsibility in this project, but remains interested in it as it was a consequence of CHEMRAWN VII. Dr Pariser agreed to continue his role as co-ordinator.

CHEMRAWN VIII

Due to the instability of Russia, no printed documents have been forthcoming from the Moscow meeting.

CHEMRAWN IX, September 1996

It was agreed that the Korean Chemical Society would organize this meeting as part of the 50th anniversary of the Korean Chemical Society. The subject of the meeting will be, The Sustainable Production, Use, Disposal and Recycling of Materials. Four main directions were recognized for discussion, they will be treated as parallel sessions:

- Energy;
- Transportation;
- Communication;
- Construction (building materials).

UNESCO has agreed to assist in financing this meeting, particularly with regard to the costs of representatives coming from developing countries.

A number of ideas were suggested for future CHEMRAWN conferences, for example, Remediation of Polluted and Contaminated Soils, to be organized in Eastern Germany or Poland in 1997 or 1998, and perhaps a conference on Chemical Education, to attempt to improve the general awareness of chemistry amongst governments.

The next meeting of the Committee will take place in association with COCI in Guildford on August 7th 1995.

Commission on Toxicology (VII.4)

Minutes of the Commission meeting JRC Ispra, Italy, 22–24 September 1994.

Reports from scientific meetings

Dr Birger Heinzow organised, on behalf of ComToxa CTC, a symposium during the 13th International Conference on Chemical Education held in Puerto Rico, August 1994, on 'Chemical Safety and Risk Assessment' with three invited speakers, however, was unable to attend himself.

The conference aimed at improvement of chemical understanding with IUPAC COMTOX, especially, on safety in the laboratory, environmental issues, risk assessment of chemicals and basic toxicological principles. The following topics were addressed:

- How can safety in the laboratory be improved and how can this be taught at different levels of chemical education?
- What is risk assessment and how is it performed.
- Environmental education in school chemistry – chemical experiments without waste production.

Prof. Templeton reported on the Vth International Conference on Nickel Metabolism and Toxicology, Sudbury, Canada held on 7–12 September 1992. The Proceedings were published in a special issue of the *Science of the Total Environment*, **148**, (2,3) 1994, under the heading 'Nickel biochemistry, toxicology and ecology issues.'

IUPAC – sponsored scientific meetings

Report on progress was received from Prof. Sunderman, Farmington (USA) who is organising the Vth ComTox Symposium on 'Chemical Toxicology and Clinical Chemistry of Metals' to be held in Vancouver, Canada, on 10–14 July 1995. The meeting will be sponsored by the Association of Clinical Scientists. Scientific sessions will be held at the Faculty of Medicine of the University of British Columbia, Canada. The International Congress of Toxicology, in Seattle, Washington, on 2–6 July 1993.

Prof. Duffas presented a brief outline of the conference on 'Carcinogenicity of Inorganic Compounds' to be sponsored by Directorate General II of the European Union with support from Eurometaux. The 4 day conference is scheduled for 17–20 October 1995 in Luxembourg. Details about the conference will be given later. A draft program has been prepared and IUPAC sponsorship will be requested.

The symposium will address the health significance of dust and particulate on the respiratory system, with state of the art lectures followed by workshops.

Dr Enrico Sabbioni presented the latest results of his research unit and reported on the 'state of the art' of the Chromium Reference Value Study. This is part of the long-term development of reference intervals for trace elements and organic compounds, in co-operation with the EURO-TERVITH program and the Tracy-Project. In Italy, a society with 150 members has been formed with the aim of studying reference intervals. It's activities cover working parties, regular conferences and the planning of a scientific journal.

The *IUPAC Glossary of Terms in Toxicology* published in *Pure & Appl. Chem.*, **65** (9), pp. 2003–2122,

1993, will be translated into Spanish. This ComTox-activity has been received with great interest by WHO and IPCS, who are already using the material for educational purposes. At present, the suggested expansion on Terms in Ecotoxicology and co-operation with SETAC (Society for Environmental Toxicology and Chemistry) is under discussion and pursued by Dr Duffus.

In line with the project to expand some of the terms for advanced education and training together with CTC, a draft proposal for Educational material, introductory level, '*Extended Educational Material for Undergraduate Training of Chemists in Toxicology*' has been prepared by Dr Duffas and Dr Howard Worth. Authors for the chapters have been assigned and the first manuscripts have been received. The quality of the submitted papers is up to expectation and it is expected the first draft of 200–250 pages will be completed by spring 1995.

'*Calculation and Application of Confidence and tolerance Intervals*'. Dr J. Molin Christensen outline the status of the project and the use of the term coverage interval. In her latest draft, the topic was simplified for the non statistician. This well-defined statistical approach offers the advantage to use valid approximations with low sample numbers and describe their uncertainties or predict the certainty of future observations. It was recommended to use in general non-parametric intervals.

Prof. Marek Jakubowski discussed the first draft of '*Sampling Strategy for Reassessment of Internal Exposure with Volatile Organic Chemicals*', particularly the problems and pitfalls of biomonitoring VOCs in the environmental and occupational setting. There is a lack of data to link dose and health outcome and to establish basic understanding on the pharmacokinetics of many compounds. Dr Jakubowski also questioned the value of 'end of workshift' sampling and exhaled air measurements. In the first draft he has mainly dealt with the kinetic problems of biomonitoring for VOCs (sampling protocol, time of exposure, time of collection). Dr B. Heinzow and Dr Dawling have prepared a chapter on the sampling technique (pre analytical and analytical precautions) as part of the project.

It was recommended to develop a curriculum for Toxicology for Chemists to be included in their regular education. CTC should take the lead of this project, and ComTox will offer assistance.

Because of the excellent co-operation between IUPAC, ComTox and IUTOX during the preparation of the Glossary it was suggested to include IUTOX in the project on Education material '*Extended educational material for undergraduate training of chemists in toxicology*'.

Future task of the Commission of Toxicology were discussed in the light of the latest proposal by Prof. Steyn in a letter to Prof. Peter Lehman. The commission discussed the remarks of Prof. Steyn related to risk assessment. It is the opinion that the commission is already dealing with many aspects of this topic and it strongly endorses involvement in this direction. It appears, however, that comments in this regard by Prof. Steyn address the topic of hazard assessment and not of risk assessment. The commissions refer to the definitions as outlined in the IUPAC glossary of Terms in Toxicology for justification of their criticism.

Prof. D. Templeton drew the attention toward the new field of molecular biotechnology and genetic technology and the need for quality assurance. ComTox recognised this as being increasingly important and encouraged Dr Templeton to follow the development and report at the next commission meeting.

The next meeting is scheduled for 4–8 August 1995 in Guildford, Surrey (UK) during the General Assembly.

Birger Heinzow

Commission on Polymer Characterization and Properties (IV.2)

Minutes of the 19th meeting held in Akron, Ohio, USA, on 9 July 1994. A meeting was held in Akron prior to the Macro '94. The main items for discussion were the activities and plans for the working parties, but some discussion was given to future organization of the Commission with special emphasis on vice-chairmen of the working parties in order to avoid problems attendant on the absence of working party chairmen.

Working Party Reports

IV. 2.1 Structure and Properties of Commercial Plastics

This WP remains the strongest. It has now integrated both sub-groups; the East Europeans in 1992 and recently the East Asians (to be confirmed at their next research projects meeting in November 94). Therefore current membership is 73 (half from industry half from academia) with participation from 18 countries with all members active. It conducts over 15 different projects, has published 8 papers in the last 2 years and plans 10 more in the next 2 years. Some of its larger projects include studies on discontinuous fibre reinforced plastics, polymer blends and polymer mixtures and the reprocessing of PVC. It contributed 5 papers to the Macro '94 conference from activities of the WP. Three new project initiations are being planned for 1994, two on novel polymer mixtures with and without bonding interactions and another project on future requirements for the characterisation of continuous fibre reinforced composites. The WP held a meeting in Akron prior to the Commission meeting and has future meetings planned for Ja-

pan 1994, Holland 1995, and Korea 1996 (in association with the Macro'96).

IV.2.2 Molecular Characterisation of Commercial Plastics
This WP plans to hold a meeting in Europe in October 1994. It continues its activity on the molecular characterisation of polyethylene systems and also on polycarbonate.

IV.2.4 Thermal Characterisation of Polymers
The WP meets in small groups and its main theme is the collection and interpretation of data on thermal analysis with emphasis on objective data (i.e. with thermodynamic relevance) rather than 'black-box' data. It is establishing links with equipment manufacturers in order to conduct this study.

IV.2.6 Interactions of Polymers with Living Systems
Although a considerable volume of results are available from this WP and a prospect of up to 5 papers are possible, there has as yet been no final report.

IV.2.8. Modelling of Polymerization Kinetics and Processes
This WP has been restructured. Membership is at 31 but is geographically widely dispersed. The WP has two mini-workshops per year at different locations allowing its membership to remain active. The principle activity of the WP focuses around the difficult task of obtaining critically evaluated kinetic parameters and a review paper with broad contribution from the WP is planned within the next year. The WP is also embarking on a new project on control of residual monomers and oligomers where activities relating to measurement, kinetics and reduction are being planned. The WP will be holding an open forum on two occasions during the Macro'94 where it will be seeking active participation on this project.

IV.2.9. Polymer Networks
A meeting of sections of this WP is planned for Prague this summer in order to enable a start to the new project on 'smart polymers', although the Guildford General Assembly will give a greater opportunity for a larger group to pursue activity on this topic. Two other projects remain modestly active, one on elastic and viscoelastic properties of covalent networks of defined structures and the other on physical networks, however, no publications have yet emerged.

The next Commission IV.2 meeting will be held at the General Assembly in Guildford (UK) on Sunday 6 August and Monday 7 August 1995.

J. Stejskal and D. R. Moore

Commission on Thermodynamics (I.2), Subcommittee on Thermodynamic Data

Minutes of the meeting held in Clermont-Ferrand, France, 16 July 1994.

Prof. Wakeham reported on the activities of the IUPAC Thermodynamic Tables Project Centre at Imperial College, London. He said that the centre will continue to be funded for the forthcoming three years, however, at a lower level than previously. Mrs. K. M. de Reuck (Assistant Director of the Centre) will retire in September and the Subcommittee extended its thanks to her for the valuable contributions she has made to the work of the centre over many years.

Current activities

Benzene: A paper on an equation of state for the gas phase of benzene, in the form of a reduced Gibbs energy, has been submitted to *Fluid Phase Equilibria*. Development of the Helmholtz energy equation for the whole fluid surface is progressing well.

Methane: The methane volume is progressing well and a final report is expected to be ready for circulation this autumn.

Critical properties: Assessment of critical constants for inorganic substances with critical temperatures less that 400 K is continuing.

IUPAC Volume on Transport Properties: A chapter on 'equations of state', necessary in the calculation of transport properties, has been prepared.

Statue of the leader of the Gauls at Clermont-Ferrand, France.

Chemical refinery, where a knowledge of P. V. relationships for fluids are of paramount importance.

IUPAC Volume of Equations of State for Fluids and Fluid Mixtures: Mrs. de Reuck will co-author a chapter on 'Fitting equations of state to experimental data' with Prof. Wagner.

Calculating VLE for Pure Fluids: A new method has been developed for solving the equation of state to obtain solution properties.

Environmentally Acceptable Refrigerants

A report was presented to the meeting of Annex 18 of the International Energy Agency in Japan, December 1993, describing the correct behaviour of the heat capacities of pure fluids along isobars in the low-pressure gas region close to saturation.

The next International Workshop on Equations of State will be held in, or near, London in the summer of 1995, organized by Mrs. de Reuck.

A proposal to initiate a new project on carbon dioxide will be presented at the General Assembly in 1995. Other fluids of potential interest for a future study include: propane, ammonia and ethane.

Fluid Phase Equilibrium Data projects

Final Report on 1-Alkanol + n-Alkane Mixtures
Reports on outstanding parts of the project were published in a special issue of *Fluid Phase Equilibria* in August 1993. A substantial document has been sent by the Chairman to the division president and the Secretariat in Oxford. A technical report was published in *Pure Appl. Chem.* in March 1993.

Binary and Ternary Mixtures of Ethers + Alkanes + Alcohols
The project is now underway, the first workshop is a part of Session 2 (non-electrolytes) of the 13th IUPAC Conference on Chemical Thermodynamics at Clermont-Ferrand, France, July 1994.

Critical Compilations

Critical Compilation of Heat Capacities of Pure Liquids
Publication in two volumes, of order 1300 pages, expected in early 1995.

Critical Compilation of Vapour–liquid Critical Properties
Parts 1–3 have been accepted for publication in the Journal of Chemical Engineering Data. Part 4 has been submitted to the same journal. Data of unsaturated or halogenated hydrocarbons should be published in the next two parts.

Related Activities

Guide-lines for Publication of Equations of State
This project had been originally started as a Subcommittee project, but has since been taken over by Commission I.2. A draft version of the guidelines has been distributed to the Subcommittee members and generally approved.

At the previous IUPAC Conference on Chemical Thermodynamics the CCDB has expressed its willingness to assist in the production of electronic versions of STD projects where appropriate.

The next meeting of the Subcommittee on Thermodynamic Data will take place during the IUPAC General Assembly in Guildford, August 1995.

Ulrich K. Deiters (Secretary)

Commission on Spectrochemical and Other Optical Procedures for Analysis (V.4)

Minutes of the Mini-meeting held at Essen, Germany, on 17–18 September 1994.

A true European molecular spectroscopy effort

After the end of the 22nd European Conference on Molecular Spectroscopy, G. Gauglitz, D. Moore, B. Schrader and K. Volka convened a mini-meeting of Commission V.4.

We used our new found enthusiasm and understanding, particularly, after hearing the forecasts about "Spectrochemical Analysis in the 21st Century" delivered at the European Conference by the IUPAC US National Committee President Jeanette Grasselli-Brown, to make progress in three of our nomenclature documents on laser-based methods for molecular spectrochemical analysis.

Instrumentation for Dispersion: submitted for publication.

Laser-Based Molecular Spectroscopy: Fundamentals. The final version of this document was preapproved by IDCNS, and was sent to Division experts and Secretariat for comments. Synopsis will be published in Chemistry International. After 5 months of public scrutiny, all changes will be incorporated and a camera-ready manuscript will be sent to *PAC*.

Laser-Based Molecular Spectroscopy: Luminescence. The new draft prepared after the Florence mini-meeting and the Amsterdam meeting has been sent to IDCNS for approval.

Laser-Based Molecular Spectroscopy Using Scattering Processes. A latest draft was presented by Schrader. The attendees commented profusely, and another draft incorporating these changes will be circulated to Commission members by the end of the year.

Laser-Based Molecular Absorption Spectroscopy. Prof. Gauglitz presented a new version of this document. A further draft will be prepared and circulated to members for discussion and it is hoped that a final draft will be ready by the Guildford General Assembly for Commission approval.

Commission V.4 will next convene during the General Assembly, August 1995.

D. S. Moore (Secretary)

Commission on Electroanalytical Chemistry (V.5)

Minutes of the meeting held in the University of Milan, Italy, 12–13 September 1994

Reports recently published

H.P. van Leeuwen, J. Buffle, and M. Lovric, Reactant Adsorption in Analytical Pulse Voltammetry: Methodology and Recommendations, *PAC* **64**, 1015–1028 (1992).

S. Rondinini, P. Longhi, P.R. Mussini and T. Mussini, Mercury (II) oxide and Silver (I) oxide Electrodes in Aqueous Solutions, *PAC* **66** (3) 641–647 (1994).

A.K. Covington, Terminology and Conventions for Micro-electronic Ion-sensitive Devices (ISFETs) in Electrochemistry, joint project with I.3, *PAC* **66** (3) 565–569 (1994).

R. P. Buck and V.V. Cosofret, Recommended Procedure for the Calibration of Ion-sensitive Electrodes, *PAC* **65** (8) 1849–1858 (1993).

Reports in Press and Under Review by the Division Committee

R. A. Durst, R. W. Murray, R. P. Buck, K. M. Kadish and C. P. Andrieux. *Chemically Modified Electrodes: Recommended Terminology and Definitions*.

R. P. Buck and E. Linder. *Recommendation for the Nomenclature of Ion-selective Electrodes – Revised*.

P. R. Mussini, T. Mussini and S. Rondinini. *Reference Standards for pH Measurements in D_2O and Aqueous-Organic Mixtures: New Accessions and Assessments*. This document is being updated and will begin the review process with Commission V.5.

Y. Umezawa, K. Umezawa and H. Sato. *Selectivity Coefficients for Ion-selective Electrodes: Recommended Methods for Reporting K_{ij}^{pot} Values*.

Selected Active projects

Electroanalytical Biosensors: Classification and Characterization. Two versions of the document have been circulated to members of the working group on Electrochemical Biosensors and the various comments have been collected. A third draft is expected by the end of the year. In parallel, a short abstract of this work may be submitted to Biosensor and Bioelectronics.

Predicted Sensitivities for Several Techniques for Anodic Stripping Voltammetry. This document covers detection limits for stripping voltammetry, it has been evaluated in V.5 and has been sent to the Secretary of the Division for circulation.

Consistency of pH Standard Reference Values with the Corresponding Thermodynamic Acid Dissociation Constant. A new draft has been prepared and is being circulated until January 1995.

Di-oxygen Electrochemical Reduction Mediated by Complexes: Recommendations for the Analysis of Experimental Results for Reporting the Data. A first draft has been promised for circulation. Dr L'Her has asked for assistance from Prof. Fred Anson of the California Institute of Technology.

Critical Assessment of the Contribution of Liquid Junction Potentials to Analytical Potentiometric Measure-

ments: Fundamentals, Applications – including – Stability constant, Industrial and Environment. The Commission is requesting from Prof. Conington and outline covering these related parts. Clarification is being sought on the relationship of the different parts, e.g. the impact of junction potentials on general potentiometric measurements and/or specifically pH measurements.

Recommended Values for the Electrolytic Conductivity Based on Molal Solutions of Potassium Chloride. Dr Ken Pratt, NIST, USA, gave an explanation of the problems in undertaking this project, particularly curve fitting the five degree temperature increment data to continuous data at all temperatures. R. P. Buck has been authorised to write to G.S. Wilson to create a joint project between V.5 and I.3.

The next meeting of the Commission will be at the General Assembly, Guildford, in August 1995.

Klára Toth (Secretary)

Commission on Agrochemicals (VI.5)

Minutes of the meeting held in Coolfont, W. Virginia, USA, on 1–4 July 1994

Projects

20/87 Relevance of impurities in technical grade pesticides
Progress has been slow because the international companies providing data have had reservations about the possible use of these data to produce regulations for them even through contaminants are more of a problem with smaller national manufacturers. However, Dr Zeeh has agreed to review this position and a small working party will produce a short report covering some of the more important aspects for the 1995 meeting.

22/87 Off-site transport of pesticides in the aqueous phase; mathematical models for leaching and run-off
A near-final draft was tabled at the 1994 meeting. The recommendations have been approved.

26/89 The effects of storage and processing on pesticide residues in plant products
Published in *PAC*, **66**, 335–356 (1994).

27/89 Use of isolated cells to study the metabolism of agrochemicals in animals
Published in *PAC*, **65**, 2299–2312 (1993).

29/91 Agrochemicals in the air
This is a particularly important environmental project because of increased awareness that the atmosphere is an important sink for many pesticides. A range of material has been collated and chapters prepared. A full draft will be circulated by April 1995 with a more complete version will be tabled at the August 1995 meeting.

30/91 Detection and significance of biologically activated metabolites of agrochemicals in animals and man
The substantial report of this project, which is of monograph proportions, is 'in press' with *PAC*.

31/91 The disposal and degradation of pesticide waste
The resignation of Eadsforth has set back the completion of this project. However, it is regarded as an important one so a new working group has been convened to carry on the project. A change in emphasis to disposal of surplus stocks of pesticide is being made. A new draft is to be distributed for comment by March 1995 and finalised at the 1995 meeting.

32/91 Pesticide run-off: methods and interpretation of field studies
Project complete except for one section to be provided by A. Klein. Recommendations have been approved and the report will be submitted to *PAC*.

38/94 Pesticide transformation in soils in the tropics
Literature searches have been completed and a database of relevant publications produced. A draft report was tabled at the July 1994 meeting with further work carried out and a list of action items agreed for working party members.

40/94 Immunoassays for residue analysis of agrochemicals
ELISA tests are becoming widely available and this project has provided relevant guideline for their standardisation and quality control. A final report has been produced with the specialist assistance of Dr A. Krotsky, BASF Gmbh.

30/93 Chirality in synthetic agrochemicals: bioactivity and safety considerations
A draft report was revised at the 1994 meeting and this revised draft will be circulated by 30 November 1994.

35/93 Environmental safety assessment for pesticides
This project is envisioned as a sequel to the major project 'Recommended approach to the evaluation of the environmental behaviour of pesticides' (Esser *et al.*; *PAC*, 60 901–932 (1980). Extensive discussions were held during the 1994 meeting regarding the scope as it needs to be held within relatively narrow limits to avoid over-committing the commission's limited resources.

However, industry, academia and agencies regards the project as extremely important. The appointment of Dr David Jones as an LT TM for this project is being sought. A draft report will be circulated by 30 June 1995.

36/93 Bound agrochemical residues in food of plant and animal origin
The scope of the project has been defined and tasks assigned for production of sections of a draft report.

Special Project: Glossary of Terms in Pesticide Chemistry
A small project has turned into a major endeavour with approximately 300 terms now gathered and put through multiple editing sessions. A near final draft is undergoing external review by about 30 authorities and IDCNS.

New projects
Projects are being considered in the following areas:
- Partition coefficients for agrochemicals (possible collaboration with Water & Soil Commission VI. 6);
- Evaluation of lysimeters – comparison with field trials and computer simulations;
- Environmental exposure assessment;
- Behaviour of pesticides in the food chain.

Workshop in Brazil, 1996

It was resolved to accept the invitations of the University of Sao Paulo (Prof. G. de Baptista), the State Department of Health and the Brazilian Society of Residue Analysts (Dr Lara) to hold a 3-day workshop in Sau Paulo in 1996, probably in October. The format will be similar to the previous successful Tianjin and Bangkok workshops with perhaps more emphasis on hands-on, practical displays. Attendance by scientists from the whole of Latin America is planned. Some funding will be provided by the Brazilian chemical industry and grants will also be sought from IUPAC and ICSU. A 3-day commission meeting would be held in Brazil immediately before the workshop. It is desirable that a commission member visit Sao Paulo during 1995 to progress planning.

Conferences

8th IUPAC Congress of Pesticide Chemistry. Washington DC, USA, 4–10 July 1994
Members involved in the organization of the scientific sessions expressed frustration at the poor communications from the US organising committee and the ACS. However, the congress went off well with over 1900 registrants and excellent conference facilities in the Sheraton hotel. A separate half-day symposium on pesticides in developing countries was also very successful.

Pesticide Chemistry for Sustainable Agriculture. Budapest, Hungary, 15–18 May 1995
This conference is being jointly organized by the Fd. Europ. Chem. Soc. and the Hungarian Chem. Soc. It is aimed at central European scientists who were unable to travel to the Washington congress. Dr Ambrus invited the commission to participate with particular emphasis on covering environmental fate of pesticides. As the full Commission must meet at the Guildford General Assembly, it proposed that 6–8 members only with expertise in environmental fate go to the meeting. A grant is being sought of $3000 as part of the IUPAC Outreach environmental programme for travel expenses of 3–4 non-industry members.

The commission will meet 5–7 August at Guildford, UK as part of the 1995 IUPAC General Assembly.

Patrick Holland (Secretary)

Commission on Atmospheric Chemistry (VI.4)

Minutes of the meeting of the IUPAC Commission on Atmospheric Chemistry, Beijing, China, on 18 July 1994.

Review of current projects

Glossary of Terms Used in Atmospheric Chemistry
Prof. Calvert proposed that this document should be reviewed and perhaps updated every four years, starting with a first review in 1995. Prof. Calvert also suggested the glossary should be sent for review to the Commission on Water Chemistry and the appropriate Commissions of the Analytical Chemistry Division. K. H. Eickel also suggested that the glossary be reviewed by OIMC, the International Organization for Metrology, Paris. It was agreed that if a great many comments, on the glossary, were forthcoming, that a subcommittee should be established to consider the various questions raised. Prof. Calvert commented that if such a subcommittee were to be created that it should include an analytical chemist and also a physical chemist.

Evaluation and Harmonization of Current Tropospherical Sampling Networks, a Collaboration with ISO
The commission has prepared a survey of existing networks and quality control recommendations. At the time, it was suggested by Dr Slanina that as ISO had a similar project, it would be reasonable that ISO took over the IUPAC project. Unfortunately, ISO has subsequently dropped their project on this topic. Consequently, the Chairman sought to contact Volker Mohnen, as co-ordinator of the workshop on Quality Assurance Planning for the Global Security Watch of the

World Meteorological Organization, to inquire if other bodies might wish to join the IUPAC effort in this area.

Evaluation and Recommendation of Units for Use in Atmospheric Chemistry
The revised document has been sent to the IUPAC Interdivisional Committee on Nomenclature and Symbols for approval.

Major Concerns and Research Needs for Our Understanding of the Chemistry of the Atmosphere
Ready for submission to *PAC*.

Evaluation and Compilation of Henry's Law Coefficients as Related to Atmospheric Chemistry
The assistance of the Commission on Solubility Data has been sought on this project.

Assessment of the Influence of Atmospheric Deposition on Water Quality
It has become apparent that this project, as it was originally envisage, would require a considerable quantity of work. Consequently, an additional titular member in atmospheric chemistry has been appointed. This new member will have the responsibility for estimating the deposition loads for South-East Asia. The Commission on Water Chemistry have made themselves responsible for preparing maps and modelling soil sensitivity. First concerns should be NO_3^- and sulfur acidification, which releases Al into the soil. The sulfate critical load

The Forbidden City in Beijing during the filming of *The Last Emperor* (courtesy of F. Cimadomo).

map for the area, although not good, is satisfactory. However, no inventories on NO_3^- emission are available.

Atmospheric Deposition of Products of Oxidation of HCFC's and Their Fate in the Hydrosphere
Prof. Calvert has contacted the Commission on Water Chemistry to enquire into the present status of knowledge on the fate of CFC's in water. Dr Slanina advised that in view of the immense amount of work this project entailed, collaborations with other ongoing projects should be established.

The next meeting of the Commission will be at the General Assembly in Guildford, UK, August 1995.

Tania M. Tavares (Secretary pro tempore)

Conferences

The 8th International Symposium on Polymer Analysis and Characterization (ISPAC-8)
22–24 May 1995
Sanibel Island, Florida, USA

This 3-day symposium will consist of poster sessions, invited lectures and round-table discussions on:

- Recent Advances in Polymer Characterization Techniques and Applications

Technical sessions will consist of:

- Polymer Separation;
- Spectroscopy;
- Scattering Techniques;
- Microscopy;
- Co-polymer Characterization.

For registration and further information, please contact: ISPAC Registration, 815 Don Gaspar, Santa Fe, NM 87501, USA, Tel: +1505 9894735, Fax: +1505 9891073.

International Conference on Chemistry and the Mediterranean Sea
23–27 May 1995
Taranto, Italy

The conference will deal with some aspects of chemistry related to the Mediterranean Sea, primarily with waste-waters and remediation of coastal waters. The following topics will be specifically addressed:

- Biogeochemical cycles;
- Environmental contamination;
- Quality of coastal waters;
- Petroleum, sea and coastal areas;
- Plastics and the sea;
- Environmental data-bank.

Panels on the effects of regulatory actions, as well as on innovations in the chemical industry for a sustainable development are planned.

An exhibition of instrumentation, environmental tech-

nology, books and scientific publications will be organized in the conference area.

Further information may be obtained from: Professor Pietro Tundo, Inter-University Association, Chemistry for the Environment, Department of Environmental Sciences, University of Venice, Dorsoduro 2137, 30123 Venice, Italy.

The 5th COMTOX Symposium on Toxicology and Clinical Chemistry of Metals 10–13 July 1995 Vancouver, Canada

IUPAC SPONSORED

The Vth COMTOX Symposium will be held at the University of British Columbia on 10–13 July 1995, in the week between the VIIth International Congress of Toxicology in Seattle, USA, and the American Association for Clinical Chemistry meeting in Anaheim, California, USA. The symposium is a satellite meeting of the International Congress of Toxicology.

The University of British Columbia was chosen as the site for the COMTOX Symposium, because it has an outstanding programme in metal toxicology, extensive instrumentation for activation analysis of metals at its TRIUMF facility, and active research projects on trace metals in relation to nutrition, molecular biology, pathology, pharmacology, genetic disease, occupational medicine and environmental health.

The four major themes of the symposium are:

1 Analysis of metals in biological materials, modern techniques for analysis of metals in biological systems.

2 Molecular biology and toxicology of metals, cellular entry and sub-cellular translocation of metals; metal-binding to macromolecules and diffusible ligands; metals in cell division, gene replication and transcription; metal-induced free radical reactions; mechanisms of metal genotoxicity, carcinogenesis and teratogenesis.

3 Metals in health and disease, metals absorption, distribution, and kinetics; animal models; dietary requirements; toxicity for various organs; genetic disorders of metal metabolism; metal accumulation in organ insufficiency; metal compounds as drugs and chemotherapeutic agents; chelation treatment and dietary therapy for metal overload.

4 Occupational and environmental exposures, chemical and biological monitoring of metal exposures from occupational, environmental, and iatrogenic sources; metal release from dental and orthopaedic prostheses; biomarkers of metal toxicity and carcinogenesis; epidemiological studies.

There will be eight full plenary lectures, and shorter presented papers. There will also be poster presentations. The official language will be English.

The registration fee, for everyone excepting accompanying persons, after 15 January 1995 will be USD450. There will be a symposium dinner at USD50 a ticket, and a harbour cruise and barbecue at USD75 a ticket.

The COMTOX symposium has reserved a large block of single and double rooms for registrants and accompanying persons in a student residence on the UBC campus. The room rate will be CAD 32 per night (plus 15% tax) for a single room with shared facilities. A double room will be CAD 70 per night (plus 15% tax). These prices are for accommodation only and do not include meals. If you wish to stay on campus, you should contact the University of British Columbia Conference Centre, 5961 Student Union Blvd., Vancouver, BC, Canada V6T 2C9, Tel: +1604 8221010, Fax: +1604 8221001.

For further information contact: F. William Sunderman Jr MD, Association for Clinical Scientists, PO Box 1292, Farmington, CT 06034-1292, USA, Tel: +1203 6792 328, Fax: +1203 6792154

36th Microsymposium on Macromolecules, High-Swelling Gels 10–14 July 1995 Prague, Czech Republic

IUPAC SPONSORED

The venue for this microsymposium will be the Institute for Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague.

The Microsymposium will bring together theoreticians and experimentalists in the field of natural and synthetic hydrogels. Thereby, affording an opportunity for the exchange of ideas and results of investigations

Vancouver.

of hydrogels with the aim of making use of the findings in fields as diverse as medicine, biology and pharmacy. The investigation of transport properties of hydrogels and their interaction with biologically active molecules will also be included.

Topics for discussion include:

- chemistry of natural and synthetic hydrogels;
- physico-chemical and transport properties of hydrogels;
- surface interactions of hydrogels with living tissue
- encapsulation of pharmacologically and biologically active substances in hydrogels;
- drug delivery systems.

It is foreseen that there will be 12 invited lectures, 20 shorter special lectures, together with poster sessions. A panel discussion on new polymer applications will be organized, the invited panel discussion-leader will be Professor W. Ringsdorf (Johannes-Gutenberg-Universität, Mainz, Germany). The conference language will be English.

The full registration fee, which includes lunches, will be CHF450 with a fee of CHF150 for accompanying persons. Accommodation will be available in student hostels within easy reach of the conference centre by public transport. The cost of accommodation is not included in the registration fee.

Prague is one of the great cities of Europe. For a time it was the capital of the Holy Roman Empire, when one of the Emperors, Rudolf II, was suspected for his interest in alchemy. The castle, which dominates the city, was the scene of the 'defenestration' of the two Imperial Commissioners Martinez and Slavata by the Protestant nobles of Bohemia which started the Thirty Years War in 1618. More recently, the Czech composer Smetana was inspired by the castle for one of his *Ma Vlast* pieces. The city boasts some of the finest medieval architecture in Europe which due to its isolation during the Cold War has remained untouched by western-style development. The old town contains unique Gothic architecture, including the oldest university in central Europe, Charles University.

Further information may be obtained from: P. M. M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic.

38th IUPAC General Assembly, Guildford '95

IUPAC General Assemblies are held in odd-numbered years. The next such assembly, the 38th General Assembly, will take place in Guildford, UK, during August 1995.

Invitation to Affiliates to attend the General Assembly

On the occasion of the 38th IUPAC General Assembly, Affiliates are invited to participate, as observers, in the meeting of the IUPAC bodies in whose work they are interested. The names and addresses of the Chairpersons of IUPAC bodies were published in *Chem. Intl.* **15**, 216–227 (1993) and subsequent issues will contain details of any changes of address.

Advance approval of the Chairperson of the relevant body should be sought and obtained before an observer may attend a meeting; a copy of the letter should be sent to the IUPAC Secretariat. Copies of Chairpersons' replies should also be sent to the IUPAC Secretariat, and if permission is granted the Affiliate observer will be sent the Information Booklet, Accommodation Reservation Form, etc. so that attendance may be confirmed to the IUPAC Secretariat.

36th IUPAC International Symposium on Macromolecules IUPACMACROSEOUL '96 Seoul, Korea 4–9 August 1996

IUPAC SPONSORED

The first circular for this IUPAC sponsored conference has just been published. The conference will be held in Seoul in August 1996, the venue has not yet been finalized. The meeting commemorates the 20th anniversary of the Polymer Society of Korea.

Plenary lectures, invited lectures, and contributed papers will cover the following sessions:

- polymer synthesis and reaction;
- polymer structure and properties;
- thermodynamics and molecular dynamics;
- polymer processing;
- polymer blends and composites;
- polymer membranes;
- field responsive polymers;
- bio-related polymers;
- supramolecular assembly and polymer thin films;
- polymers and the environment;
- polymer education.

Early registration (before 1 March 1996) for a full participant will be USD500 and USD75 for a student and accompanying person. Later registration will be USD550 and USD100, respectively.

Further information can be obtained from: Dr Kwang Ung Kim, Secretariat IUPACMACROSEOUL'96, Division of Polymers, Korea Institute of Science and Technology, PO Box 131, Cheongryang, Seoul 130–650, Korea (Tel: 82 2 957 6104 Fax: 82 2 957 6105 E-mail: iupac@kistmail.kist.re.kr).

Eighth IUPAC Symposium on Organometallic Chemistry directed towards Organic Synthesis. OMCOS 8. 6–10 August 1995 Santa Barbara, California, USA

IUPAC SPONSORED

The 8th IUPAC Symposium on Organometallic Chemistry directed towards Organic Synthesis will take place next August in Santa Barbara, California.

The aims of the Symposium are the presentation of recent results, the discussion of trends, and the exchange of ideas relating to the use of metals in organic synthesis. OMCOS 8 will focus on the following topics:

- Asymmetric Synthesis via Organometals;
- Structural and Mechanistic Aspects related to Synthesis;
- Organometallics in Natural Product Synthesis;
- Metal-organics in Materials Research;
- Catalytic Processes Involving Organometallics;
- New C-C and C-Heteroatom Bond forming Processes Involving Metals;
- Cyclizations/Ring-opening Reactions Involving Organometallics.

Six plenary and 14 invited lectures are planned, as are about 15 short talks. In addition, two or three poster sessions will be scheduled, depending upon the demand, during the conference.

The official language of the symposium will be English.

A multitude of hotels are located in the greater Santa Barbara area so as to accommodate the needs of all participants.

Pre-OMCOS, a conference on Recent Advances in Organometallic Chemistry in Organic Synthesis, co-organized by Professors N. E. Shore and E. Negishi will take place at University of California Davis on 3–4 August.

Post-OMCOS, a conference on Carbanion Chemistry will be held at Colorado State University in Fort Collins, Colorado, on 12–16 August with Professor A. I. Meyers as Chairman.

The city of Santa Barbara, founded by the Spanish in the 18th Century, is considered to be one of the jewels of the Californian coast. It lies approximately 100 miles north-west of Los Angeles, nestled against the Santa Ynez mountains overlooking the Pacific Ocean. In August, the days are warm and the nights cool with occasional morning fog. Nearby are many excellent beaches, lakes, forests and mountains with varied hiking trails. Daily excursions can be made to Hearst Castle (the castle built by William Randolf Hearst – of *Citizen Kane* fame), the flower fields of Lomoc, and the Old World Village of Solvang. In Santa Barbara one can visit the Mission, the famous Courthouse, or the Botanical Gardens. Visits to these points of interest, and others, have been organized in the special tours planned for accompanying persons.

Non-technical correspondence should be addressed to: Campus Conference Services, University of California, Santa Barbara, CA 93106–6120, USA, Tel: +1805 8933072, Fax: +1805 8937287, E-mail: hr03conf@ucsbvm.ucsb.edu

Registration forms are available from: Professor Bruce H. Lipshutz, Chairman, OMCOS 8, Department of Chemistry, University of California, Santa Barbara, CA 93106–9510, USA

Santa Barbara Mission.

Energex '96

The sixth international energy forum, Energex '96, will be held in Beijing, China, 3–7 June 1996.

The theme of this meeting, hosted by the China Association for Science and Technology and the International Energy Foundation, together with support form numerous international bodies, is Energy Strategies in Developing Countries in the 21st Century: Challenges and Opportunities.

One of the many highlights will be a forum in which the United Nations Industrial Development Organization (UNIDO) programmes, projects and accomplishments, in the energy sector world-wide, will be presented and discussed.

Specialized workshops such as Active Solar Energy, Passive Low Energy Architecture, Global Climatic Change, Energy Sustainability, Photovoltaics and Science and Technology Management, will be held prior to Energex '96.

Topics for discussion include:

- Rational use of energy;
- New and renewable sources of energy;
- Environmental control and waste cycling;
- Energy policies and economics;
- Fossil fuels and clean fuel technologies.

For further information contact: Mr Liu Feng, Energex '96 Conference Manager, China International Conference Centre for Science and Technology, 44 Kexueyuan Road, Shuangyshu, Beijing, China 100086, Tel: +86 1257 5681, Fax: +86 1257 5691.

Conference Calendar

1995

Macrocyclic chemistry

2–7 July
20th International Symposium on Macrocyclic Chemistry. Jerusalem, Israel.
Prof. D. Meyerstein, Chemistry Department, Ben-Gurion University of the Negev, P.O.B. 653, Beer-Sheva 84105, Israel. Tel: +972 (7) 461238. Fax: +972 (7) 237682

Polymer morphology and electrical properties

5–7 July
International Symposium on Polymer Morphology and Electrical Properties. Lodz, Poland.
Prof. A. Galeski, Centre of Molecular & Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, 90–363 Lodz, Poland. Tel: +48 (42) 818952 or 815761. Fax: +48 (42) 847126 or 815483. E-mail: julanski@lodzl.p.lodz.pl.

Analytical chemistry

9–15 July
SAC 95: International Conference on Analytical Chemistry. Hull, UK.
Prof. A. Townshend, School of Chemistry, University of Hull, Hull HU6 7RX, UK. Tel: +44 (482) 465027. Fax: +44 (482) 466410.

Toxicology and clinical chemistry of metals

10–13 July
5th COMTOX Symposium on Toxicology and Clinical Chemistry of Metals.
Vancouver, BC, Canada.
Prof. F. W. Sunderman, Jr., Departments of Laboratory Medicine and Pharmacology, University of Connecticut Medical School, Post Office Box 1292, Farmington, Connecticut 06034–1292, USA. Tel: +1 (203) 792328. Fax: +1 (203) 6792154.

High swelling gels

10–14 July
36th Microsymposium on Macromolecules – High Swelling Gels.
Prague, Czech Republic.
P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague 6, Czech Republic. Tel: +42 (2) 360341. Fax: +42 (2) 367981. E-mail: sympo@imc.cas.cz.

Functional dyes

16–21 July
3rd International Symposium on Functional Dyes (Functional Dye '95). Santa Cruz, California, USA.
Dr J. Pacansky, IBM – Almaden Research Center, K42/803, 650 Harry Road, San Jose, CA 95120–6099, USA.

Heteroatom chemistry

30 July – 4 August
4th International Conference on Heteroatom Chemistry. Seoul, Korea.
Prof. Kyongtae Kim, Secretary General, ICHAC-4, Department of Chemistry, Seoul National University, Seoul 151–742, Korea. Tel: +82 (2) 8806636. Fax: +82 (2) 8748858.

Novel aromatic compounds

31 July – 4 August
8th International Symposium on Novel Aromatic Compounds (ISNA-8). Braunschweig, Germany.
Prof. H. Hopf, Institut für Organische Chemie, Technische Universität, Hagenring 30, D-38106 Braunschweig, Germany. Tel: +49 (531) 391 5255. Fax: +49 (531) 391 5388

IUPAC General Assembly

4–11 August
38th IUPAC General Assembly. Guildford, Surrey, UK.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion

Organometallic chemistry directed toward organic synthesis

6–10 August
8th IUPAC Symposium on Organometallic Chemistry directed toward Organic Synthesis (OMCOS-8). Santa Barbara, California, USA.

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* **14**, 203 (1992).

Prof. B. H. Lipshutz, Department of Chemistry, University of California, Santa Barbara, California 93106–9510, USA. Tel: +1 (805) 8933072. Fax: +1 (805) 8937287. E-mail hr03conf@ucsbvm.ucsb.edu.

Heterocyclic chemistry

6–11 August
15th International Congress of Heterocyclic Chemistry. Taipei, Taiwan, China.
Prof. Chin-Kang Sha, Department of Chemistry, National Tsing Hua University, Hsinchu 300, Taiwan, China. Tel: +86 (35) 722427. Fax: +86 (35) 725870. E-mail: cksha@chem.nthu.edu.tw.

35th IUPAC Congress

14–19 August
35th IUPAC Congress. Istanbul, Turkey.
Prof. A. Riza Berkem, Halasgargazi Cad. No. 53, D. 8, 80230 Harbiye, Istanbul, Turkey. Tel: +90 (212) 2407331. Fax: +90 (212) 2317037.

Plasma chemistry

21–25 August
12th International Symposium on Plasma Chemistry. Minnesota, Minneapolis, USA.
ISPC-12, c/o Catherine Ploetz, 218 Nolte Center, University of Minnesota, 315 Pillsbury Drive SE, Minneapolis, MN 55455, USA. Tel: +1 (612) 6262259. Fax: +1 (612) 6261632. E-mail: ispc12@pdcs.cee.umn.edu

Spectroscopy

27 August – 1 September
29th Colloquium Spectroscopicum Internationale. Leipzig, Germany.
CSI XXIX Secretariat, Gesellschaft Deutscher Chemiker, Abt. Tagungen, Postfach 90 04 40, D-60444 Frankfurt am Main, Germany. Tel: +49 (69) 7917358. Fax: +49 (69) 7917475.

Liquid and amorphous metals

27 August – 1 September
9th International Conference on Liquid and Amorphous Metals. Chicago, USA.
Drs Saboungi and Price, Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA. Tel: +1 (708) 252 4341 (M.-L. Saboungi), +1 (708) 252 5475 (D. L. Price). Fax: +1 (708) 252 7777 (both)

Industry – education initiatives in chemistry

28 August – 2 September
International Symposium on Industry – Education Initiatives in Chemistry. York, UK.
Dr J. F. Gibson, The Royal Society of Chemistry, Burlington House, Piccadilly, London WIV OBN, UK. Tel: +44 (0)71 4378656. Fax +44 (0)71 7341227.

Solution chemistry

29 August – 3 September
24th International Conference on Solution Chemistry. Lisbon, Portugal.
Prof. César A. N. Viana, CECUL – Faculdade d· Ciencias, Universidade de Lisboa, R. Escola Politécnica, 58, 1294 Lisboa Codex, Portugal. Tel: +351 (1) 608823. Fax: +351 (1) 7977837

Medicinal chemistry

3–8 September
AFMC International Medicinal Chemistry Symposium (AIMECS 95). Tokyo, Japan.
Prof. S. Ikegami, Secretary General, AIMECS 95, c/o Faculty of Pharmaceutical Sciences, Teikyo University, Sagamiko, Kanagawa 199–01, Japan. Tel: +81 (426) 850161. Fax: +81 (426) 851870.

Ionic polymerization

4–8 September
1st International Symposium on Ionic Polymerization. Istanbul, Turkey.
IUPAC International Symposium on Ionic Polymerization, c/o Prof. Y. Yagci, Istanbul Technical University, Faculty of Science, Department of Chemistry, Maslak 80626, Istanbul, Turkey. Tel: +90 (212) 285 32 41. Fax: +90 (212) 285 63 86. E-mail: Feyusuf@TRITU

Applications of the Mössbauer effect

10–16 September
International Conference on the Applications of the Mössbauer Effect (ICAME-95). Rimini, Italy.
Prof. I. Ortalli, University of Parma, Istituto di Scienze Fisiche, Via M. D'Azeglio, 85, 43100 – Parma, Italy.

Bioorganic chemistry

17–23 September
3rd International Symposium on Bioorganic Chemistry. Dagomys, Sochi region of Black Sea Coast, Russia.
Dr V. V. Demin, Shemyakin – Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Ul. Miklukho-Maklaya, 16/10, 117871 Moscow V-437, Russia. Tel: +7 (095) 3351511, 330–6338, 3302800. Fax: +7 (095) 3107007.

Chromatography of polymers

18–22 September
International Symposium on Chromatography of Polymers and Related Substances. Bratislava, Slovakia.
Dr D. Berek, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, Sk-842 36 Bratislava, Slovakia. Tel: +42 (7) 3782306. Fax: +42 (7) 375923.

International Union of Pure and Applied Chemistry (IUPAC)

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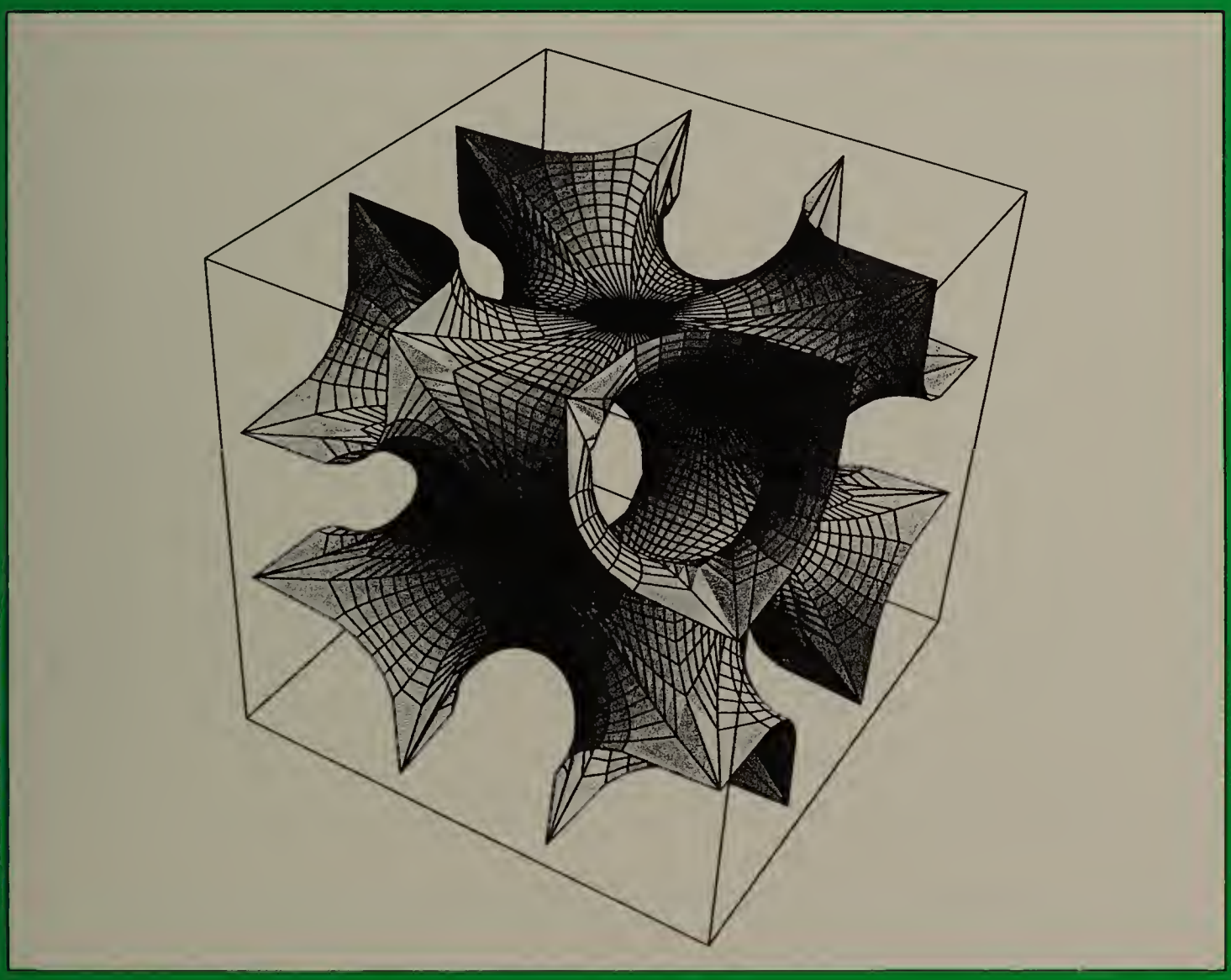

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Front cover: A generated minimal surface. This structure is a representation of the solution of a particular set of mathematical equations.

International Union of Pure and Applied Chemistry

Clinical chemistry: an interface between chemistry and medicine

H. Peter Lehmann

Clinical chemistry is the body of chemical knowledge that is used by scientists and physicians to investigate disease processes in man. Its practitioners use knowledge of physical chemistry to explain pathophysiological processes, organic chemistry and biochemistry to explain metabolic processes, and analytical chemistry to measure changes in the pathophysiological and metabolic processes that are associated with health and disease.*

Looking through the topics discussed in the most recent periodic review of clinical chemistry in *Analytical Chemistry*[1] (Table 1) reveals the diversity of activities which are considered to lie in the realm of clinical chemistry. The specific topics are divided into two categories; clinical and instrumental, which reflect the major areas of activity of the speciality. Included in the instrumental section is management, relating to quality processes implemented in the laboratory to ensure clinically relevant data is generated for patient care.

In its most recent report on world health, the World Health Organization (WHO) lists cardiovascular diseases and cancer as the number one and two disease problems in developed countries, while these take places two and four, respectively, in health problems in less-developed countries.[1]

In spite of a great deal of knowledge and understanding of many of the risk factors associated with cardiovascular disease (CVD), for example dyslipidermia, smoking, hypertension, obesity, diabetes, lack of exercise and stress, and the medical interventions necessary and life-style changes recommended for individuals at risk, CVD remains a significant worldwide health problem. Jacobsen[2] reviews the current status of two independent risk factors for CVD; lipoprotein (a) [Lp(a)] and homocysteine. Because of structural homology of significant segments of Lp(a) and plasminogen (a protein intermediate of the blood clotting reaction cascade), and known competition between Lp(a) and plasminogen for binding sites on blood cells and vascular endothelial cells, it is thought that high-levels of Lp(a) can enhance thrombotic and coagulant properties of the cells, resulting in CVD. Jacobsen describes immunoassays for Lp(a) that have been developed and used to test the Lp(a) hypothesis. The observed associations between Lp(a) and clinical disease led Jacobsen to suggest that standardization of Lp(a) assays are needed (a current project of the International Federation of Clinical Chemistry), and to speculate that determination of Lp(a) isoforms and their association with disease could lead to gene-therapy as an approach to the reduction of this risk factor for CVD. Jacobsen also reviews the evidence for the association between homocysteine and CVD. A metabolite of methionine metabolism, homocysteine has been implicated in the etiology of CVD arising from injury to endothelial cells. With the development of reliable assays for homocysteine in the blood, numerous studies have raised questions concerning the role of the amino acid in atherogenesis and the genetic control of its synthesis and catabolism, and how these may be modified to reduce risk for CVD. Finally, Jacobsen suggests that the two components, Lp (a), and homocysteine, may be linked risk factors due to the effect of the amino acid on

*'Health' and 'disease' are antonyms. While clinical chemists have traditionally served physicians in the management of their patients (disease), they are increasingly applying their knowledge to the maintenance of health (non-disease) through activities in the area of preventative medicine by screening for risk of disease.

Table 1. Review Topics in Clinical Chemistry (taken from reference 1)

Clinical	Instrumental
Cardiovascular disorders	Molecular biology techniques
Free radicals	Immunoassays
Endocrine disorders	Capillary/ electrophoresis
Cancer	High performance liquid chromatography
Bone disorders	Clinical instrumentation
Acquired immunodeficiency syndrome	Electroanalysis and biosensors
Diseases of metabolism	Fluorescence spectroscopy
Psychological disorders	Chemiluminescence and bioluminescence
Electrolytes and blood gases	Flame, flameless and plasma spectroscopy
Therapeutic drug monitoring	Mass spectrometry
	The National Reference System
	Statistics

Lp (a) structure. The association between homo–cysteine and CVD is also reviewed by Kazmierczak[1] in discussing diseases of metabolism, specifically amino acids. The significance of this review is affirmed by the recommendation of the WHO Scientific Group on Cardiovascular Disease Risk Factors, which recommends research on new and simplified technologies to identify atherogenic lipoproteins, including Lp (a), and to determine the relevance of high levels of homocysteine in populations as a marker of risk for CVD.[3]

In the review of clinical chemistry and cancer, Katzin restricts himself to a discussion on the role, measurement and disease associations between paraproteins and lymphoproliferative diseases, such as multiple myeloma, non-Hodgkin's lymphoma, plasmacytomas and amyloidosis.[1] Paraproteins are monoclonal immunoglobulins synthesized and secreted by specific clones of B-lymphocytes, that are thought to be important for the clonal nature of some cancers. Therefore, its reliable detection and measurement is significant for the diagnosis and monitoring of lymphoproliferative diseases. Katzin discusses the electrophoretic procedures used to identify and quantify specific immunoglobulins. Although the prognostic implications of measuring paraproteins are still inconclusive, Katzin presents information which suggests that, at this time, the quantification of β-2 microglobulin offers some clinical possibilities.

The number one health problem in less-developed countries is infectious diseases which, in spite of advances in public health programs and the availability of antibiotics, continue to be the major cause of high infant mortality and hence low overall life expectancy. The last decade has witnessed the explosive world-wide progression of one infectious disease; acquired immunodeficiency syndrome, with devastating results particularly in less-developed countries. For example, it is estimated by WHO that 9 million adults are infected with the causative virus (HIV) in Sub-Saharan Africa.[4] The review by Proffitt describes areas in which clinical chemists help to address this world-wide medical problem, by reviewing the current status of HIV antibody and antigen immunoassays.[1]

Immunoassays play a key role in the practical application of all the clinical topics discussed. This type of assay is defined by Hage as the technique which uses antibodies or antibody related reagents for the selective determination of sample components.[1] The adaptability of the technique and its selectivity, sensitivity and low limits of detection are cited as factors that make it particularly helpful for clinical use. Developments in procedures for antibody production, leading to improved selectivity for the analytes to be measured, and in procedures for labelling (with radionuclide, enzyme, fluorescent, and chemiluminescent tags) that result in improved sensitivity are reviewed. The introduction of non-isotopic labels for immunoassays opened the way for automation of the assays. This is described by Haas, who compares the features and operating characteristics of 19 systems currently on the market.[1] He also discusses some of the practical factors that must be considered in using such systems for clinical purposes. These are issues that must be addressed by clinical chemists to ensure the quality of the services offered by the laboratory to their clients (physicians and patients) is maintained. Until recently one of the often stated advantages of radioimmunoassay included the sensitivity of the method. Replacement of radionuclide labels with fluorescent and chemiluminescent labels with improved sensitivity, down to zeptomole (10^{-21} mole) amounts, is another major advance in immunoassay technology that is reviewed by Diamandis (fluorescence)[1] and Kricka (chemiluminescence and bioluminescence).[1]

Use of similar detection systems in DNA binding analytic techniques have led to the development and application of DNA probe technology to clinical practice. Combined with *in-vitro* techniques to amplify DNA from biological samples, for example the polymerase chain reaction, molecular biology technology is being introduced into the clinical laboratory, particularly for the diagnosis of genetic diseases and some cancers and for the detection of infectious disease agents. Such clinical use is still new and in an experimental stage with, as Skogerboe[1] points out, issues of quality assurance, cost, and patient privacy still to be resolved. Nevertheless, the application of recombinant DNA techniques to the detection of genomic material (endogenous and exogenous) for the diagnosis of disease is increasing, and has given rise to a number of 'molecular' medical specialities, for example molecular genetics, molecular pathology and molecular diagnostics, that all have nucleic acid chemistry as their basis.

Immunoassays and DNA probe assays represent an 'expansion' of clinical chemistry into areas outside the traditional sphere of activity of the speciality, for example into genetics, microbiology, immunology and virology. This expansion of activity is clearly illustrated by the role, over the years, of the clinical laboratory in the detection and management of viral hepatitis in patients (Table 2). The association between infection by hepatitis B virus (HBV) and hepatocellular carcinoma has been well documented in epidemiological studies.[5] It has been estimated that world-wide there are ~ 300 million active carriers of the HBV. In less-developed countries 10–20% of these become chronic carriers, and 30–40% of these persons advance to cirrhosis of which 10–40% progress to hepatocellular carcinoma. Although in developed countries the figures are lower (0.5% chronic carriers of which 25% develop cirrhosis and 5% hepatocellular carcinoma), HBV infection and its consequences represents a significant world-wide

Table 2. Laboratory diagnosis of viral hepatitis

1950- metabolic products/ enzymes:	1970- viral antigens/ antibodies: *	1990- viral DNA/RNA: *
t-bilirubin transaminases: AST/ALT	anti-HAV: IgM anti-HAV: IgG	HAV-RNA
	HBsAg HBeAg anti-HBs anti-HBe anti-HBc: IgM anti-HBc: IgG	HBV-DNA
	anti-HCV	HCV-RNA HDV-RNA HEV-RNA
Spectrophotometric assays	Immunoassays	Nucleic acid hybridization assays

* HAV hepatitis A virus
HBV hepatitis B virus
HCV hepatitis C virus
HCD hepatitis D virus
HEV hepatitis E virus

anti- antibody to
Ag antigen
IgM immunoglobulin M
IgG immunoglobulin G
Hbs hepatitis B surface (antigen)
HBe hepatitis B e (antigen)
Hbc hepatitis B core

health problem. Prior to 1970, inflammatory disease of the liver (hepatitis) was diagnosed through chemical, colorimetric-based assays for bilirubin and liver enzymes. While appropriate use of test combinations permitted a differential diagnosis of the disease physicians often had to rely on patient history to determine the cause of the problem. The discovery, in 1965, that inflammatory disease of the liver could be caused by a virus (HBV) was quickly followed by the development of immunologically based laboratory tests that determine the presence of viral antigens and antibodies in samples from infected patients. An important aspect of these tests is their diagnostic sensitivity, that is their availability to detect the infection or the biological consequences of infection through viral antigens and antibodies in patients. However, cases of HBV infection are still missed by traditional radioimmunoassays because they lack the analytical sensitivity to detect very small levels of virus particles. This problem has been addressed by developing more analytically sensitive detection systems for immunoassays[1] or by developing alternate detection and measurement systems.

The latter has occurred with use of direct DNA hybridization assays in conjunction with the polymerase chain reaction for the detection of HBV-DNA. Such a procedure permits detection of ~ 10^3 viruses per milliliter of sample.[6] As already indicated, chronic hepatitis B is frequently the initial step in the development of hepatocellular carcinoma.[5] Using DNA hybridization techniques a differential diagnosis of chronic hepatitis B carrier status can be made between the 'healthy' asymptomatic carrier (< 10^5 HBV-DNA viruses per milliliter) and non-replicative chronic hepatitis patients (> 10^5 HBV viruses per milliliter). Individuals in the latter group are candidates for (costly) interferon alpha therapy to prevent progression to cirrhosis and hepatocellular carcinoma. In this way, a combination of chemical, immuno- and molecular biology assay techniques can play a significant role in reducing the incidence or cirrhosis and hepatocellular carcinoma.

The term 'molecular epidemiology' was coined in the early 1980s to describe research that was being conducted to elucidate mechanisms between the cause and effect observations of traditional epidemiology. For example, through classical epidemiology a number of causative agents have been associated with gastric tissue changes that ultimately lead to gastric cancer (Figure 1).[7] Studies using molecular biology techniques have complemented the epidemiological model for gastric cancer and have provided information on genomic changes in precancerous gastric tissue (Figure 2).[7] Such molecular biology studies will enable clinical chemists to play a role in the diagnosis and prevention of this world-wide health problem. Analyzing gastric fluid for acidity (pH), nutritional deficiencies (anti-oxidants, carotenoids), and carcinogens (nitrates and nitroso-compounds), and gastric tissue for genomic changes will provide objective information that can be used to initiate preventative therapies. For example, it has recently been shown that treatment of *Helicobacter pylori* (*H. pylori*) infection (a risk factor for gastric cancer) results in a six-fold increase in total vitamin C (ascorbic acid + dehydroascorbic acid), an antioxidant, in the stomach.[9] This leads to protection of cells from oxidative changes that occur as a result of chronic inflammation due to *H. pylori* infection. In another study, alterations of the p53 gene (a tumour suppressor gene) at different stages of gastric tissue transformation leading to cancer were investigated. [10] Using the polymerase chain reaction to amplify p53 exons 5–8 followed by single strand conformation polymorphism and DNA sequencing, gene alterations were found at the metaplasia stage (38% of cases), the dysplastic stage (58%) and in carcinoma (67%). Because gastric cancer is often not diagnosed until it reaches an advanced stage, use of tests such as those described as part of the diagnostic process for chronic gastritis could lead to improved prevention of this deadly form of cancer.

Table 3: Epidemiology of Gastric Cancer

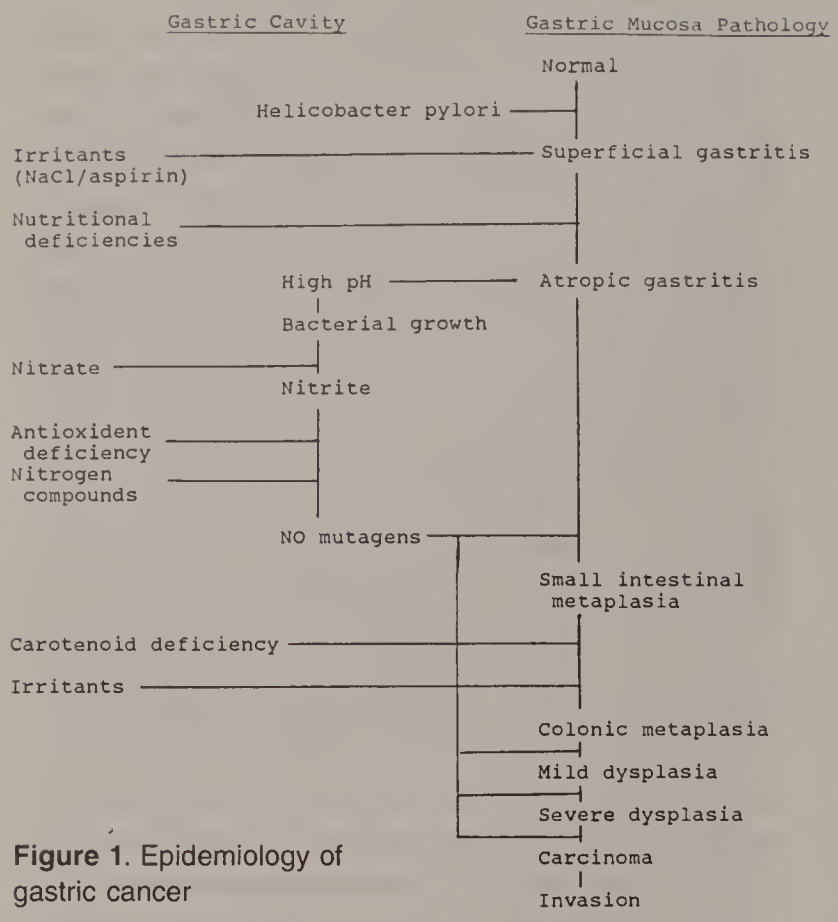

Figure 1. Epidemiology of gastric cancer

These are just a few examples of the many avenues for development of clinical chemistry. Recently the United States National Institute of General Medicinal Science (NIGMS), a major source of funding for biomedical research in the United States, has listed areas of interest.[11] Included are biotechnology, human medical genetics, mechanisms of mutagenesis, molecular immunobiology, replication, recombination and repair of genes, neurogenetics and genetics of behavior. All of these when applied to human health fall into the realm of molecular pathology, which, as described, has chemical techniques and procedures as its basis. Amongst other areas of interest to the NIGMS that have a distinct chemical nature are analytical and separation techniques, membrane structure and function, spectroscopic techniques, bioorganic and bioinorganic chemistry, medicinal chemistry and synthetic chemistry. As fundamental research findings in these areas are applied directly to patient care, clinical chemists will have a role to play to ensure the data generated in the laboratory meet the rigid criteria necessary to ensure their appropriate utilization.

The role of IUPAC in these developments is in the area of international standardization of nomenclature, technologies and procedures, and in the formulation of quality management standards for laboratories involved in such testing. The recently completed and current ongoing projects of Commissions VII.2 and VII.4, as well as Limited Lifetime Commissions and Working Groups of the Clinical Chemistry Division,[12] will serve as models for future IUPAC programs in the general area of chemistry and human health.

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Table 4: Molecular Epidemiology of Cancer

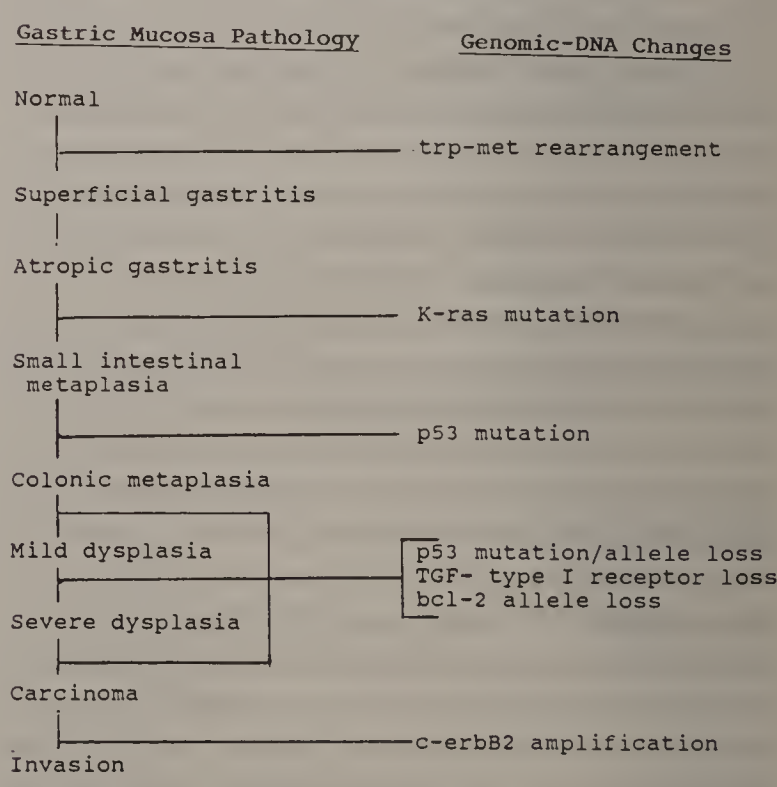


Figure 2. Molecular epidemiology of cancer

Molecular Electronics

Organic semiconducting materials, such as conjugated polymers and oligomers, have recently been used as active components in electronic devices such as field-effect transistors and electroluminescence diodes (LEDs). Now, Francis Garnier (Laboratoire des Matériaux Moléculaires, Thais, France) and co-workers (*Science* 265, 1684 (1994)), by using organic compounds as substrates and contact electrodes, have developed an 'all plastic' electronic device. Thereby creating the attractive perspective of low-cost and large-area fabrication of mechanically flexible electronics.

The active layer in Garnier's device is di(hexyl) sexithiophene of 40 nanometer thickness, with high resistive layers of polyethylene terephthalate as a substrate and a conducting graphite polymer ink as a means of achieving electrical continuity. This is the first truly 'all plastic' device as previous organic semiconducting materials had to be connected to metallic (gold or calcium) source and drain electrodes.

Light-emitting diodes (LEDs) are well known, however, the use of polymers as the active component in an LED is at the forefront of today's technology.

The range of different materials now available for polymer-based LEDs is such that electroluminescence can now be obtained throughout the visible spectrum. By blending polymers with different emission and charge-transfer characteristics, LEDs can be fabricated in which the emission colour varies as a function of the applied operating voltage. This phenomenon arises from the self-organizing properties of the polymer blends, in which entropy drives phase separation of the constituent polymers and gives rise to submicrometer-sized domains having a range of compositions and emission characteristics. Emission from domains of different composition is controlled by the ease with which charge carriers are injected, which is in turn determined by the applied voltage.

In a recent study by Berggren *et al.* (University of Linköping and Chalmers University of Technology, Sweden) a series of LEDs have been fabricated where the active medium is based, in each case, on thiophene incorporated into the main chain. Emission at a variety of wavelengths, from the blue to the near infrared, of the electroluminescence spectra of a series of thiophene-based polymers is observed (*Nature* **372**, 444 (1994)).

Polymer systems based on thiophene display great variability, through substitution at the 3- and the 4- position, which can be produced by 2,5-polymerization of the substituted monomer via oxidative polymerization.

The design of these polymers is carefully controlled. By altering the substitution pattern and character of the substituents, control of the torsion of the main chain and hence the conjugation length is achieved. Enhanced steric hindrance from side groups leads to a decrease in planarity of the main chain of the polymer and an increase in the band gap; simple model calculations have demonstrated that the band gap is enhanced by torsion.

The authors find that LEDs incorporating blends of these polymers allow simultaneous emission from the different polymers in the blend. For example, in certain blends blue and red emission is observed. The intensity ratio of the peaks is determined by the voltage applied to the diode, and the stoichiometry of the blend. External quantum efficiencies are in the range 0.1–1%

We are currently hearing a great deal about molecular electronics, where chemists are synthesizing and assembling new molecules which will have the electrochemical properties of very much larger pieces of inorganic semiconducting material. However, what of future developments? One of the prerequisites of a viable nanoscale device is a means of conducting the electron from one part of the nano-device to another part without it going to ground, a short circuit. That is, how do you make a nano-wire?

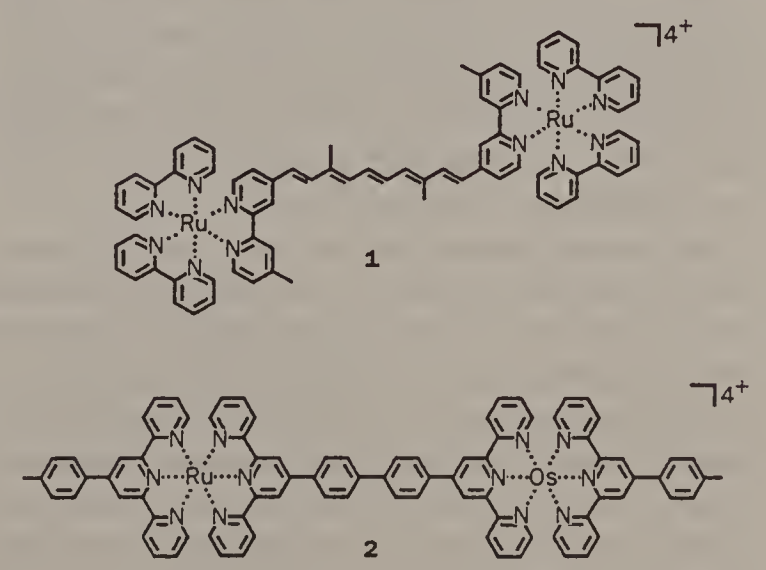


Figure 1. Transition metal complexes used in studies on molecular electronics.

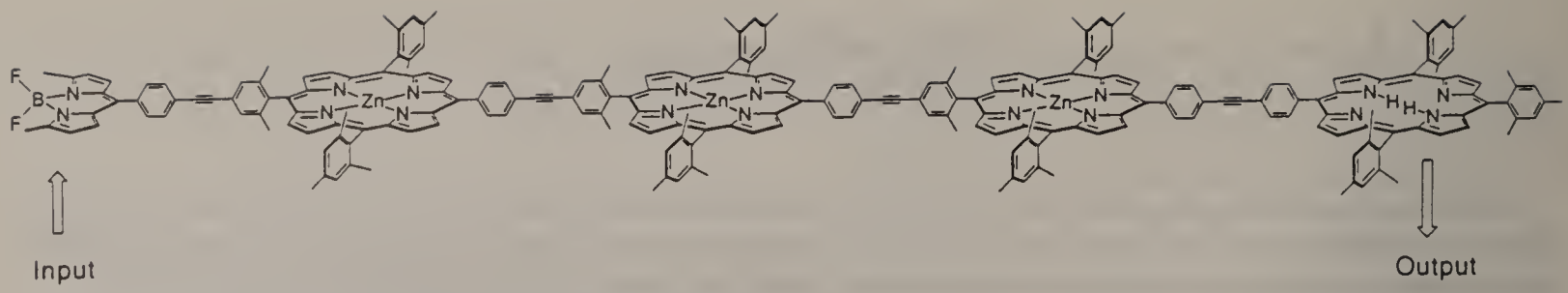


Figure 2. Molecular photonic wire is a string of porphyrins.

At a molecular level, the transfer of an electron requires overlap of donor electronic orbitals with those of the acceptor. Due to the usual atomic localization of orbitals, this desired overlap is a strong function of the distance between donor and acceptor. But the overlap can be effectively extended by incorporating an intervening material which itself overlaps with both the donor and acceptor orbitals. Molecular electricians are currently seeking nano-conductors that confer structural rigidity, preventing spatial arrangements which lead to molecular short circuits.

Prof. J.M. Lehn *et al.* have linked two metal complexes with a conjugated polyene spacer and observed long-range electron delocalization (*J. Chem. Phys.* **98**, 7798 (1994)).

The highly coloured carotenoid polyenes have long been known in photosynthesis. Photosynthetic reaction centers are molecular scale photovoltaics that carry out charge transfer across lipid membranes.

In the experiment of Lehn *et al.* the polyene spacer (5 C = C double bonds) connects two optically and electrochemically active moieties. Although separated by 24 Å, the two ruthenium complexes do not behave independently. The electronic absorption spectrum of the mixed valence (Ru^{3+}–Ru^{2+}) complex (see molecule 1 in Figure 1) shows an intervalence absorption band arising from the optically promoted transfer of charge between the metal centers. Spectroscopic data shows a strong coupling between these metal centers, which is consistent with the polyene spacer acting as a wire.

Promotion of an electron into a triplet state enhances the coupling between the two metal centers. The electron is then in an extended π-molecular orbital which itself embraces the polyene spacer.

The polyene spacer not only acts as a molecular wire, but also as a spacer. It prevents folding motions that would allow the ruthenium complexes to come into van der Waals contact. The resulting strong electronic interaction would be the equivalent of a molecular short circuit. The result of this rigidity is a stable molecular girder, rigid on the time scale of fast electron transfer.

At first sight, the work of Barigelletti *et al.* (*J. Am. Chem. Soc.* **116**, 7692 (1994)) looks similar. The ruthenium (2+) and osmium (2+) complexes are joined by a polyphenylene spacer. The structural and electronic similarities between the polyphenylene and polyene units is such as to lead one to suspect that they would behave similarly. However, steric interference between the H atoms on the adjacent phenyl rings prevents them from lying in the same plane, thus limiting conjugation. Photochemical experiments showed that the ruthenium moiety of this molecule (no. 2 in Figure 1) showed no emission at all upon excitation. Instead, only luminescence was observed from the osmium complex. This is proof of transfer of excitation energy from the ruthenium complex to the osmium complex.

Even though the Ru and Os complexes are separated by 20 Å, the observed rate of energy transfer is one thousand times faster than that for related chromophores separated by 17 Å by a rigid but non-conjugated bridge. Showing that even though the spacer is twisted there is still substantial orbital overlap, giving a molecular wire.

Again using photosynthetic apparatus as a source of inspiration, Prof. Jonathan S. Lindsey (Carnegie Mellon University, Pittsburgh, USA) has developed a molecular photonic wire 90 Å in length (*J. Am. Chem. Soc.* **116**, 9759 (1994)).

Using repetitive coupling methods. the group synthesized the photonic wire from three building blocks similar to those found in the natural photosynthetic light harvesting complexes (see Figure 2).

At one end is a boron-dipyrromethene dye which absorbs blue-green light. The resulting excitation is transmitted through the a string of three zinc porphyrins to a fluorescent metal-free porphyrin, which emits a red photon. For every 100 photons absorbed at the input, 76 excited states find their way to the output, yielding a transmission efficiency of 76%. This might seem impressive, however, the efficiency of natural photosynthesis is nearly 100%.

The wire shows features which are akin to a molecular-scale fibre-optic device. But the mechanism by which the energy is transmitted remains unclear and is under investigation.

Development of such molecular-scale electro-optic devices will usher in a new era of information processing. Potential spin-offs include molecular circuitry, artificial retinas, ultra-sensitive photoreceptors, and nanoscopic light sources.

Commission & Committee News

38th IUPAC General Assembly, 4–11 August 1995, Guildford, UK

The Commission on Biotechnology (Division of Applied Chemistry) invites all participants of the 38th IUPAC General Assembly to attend an open meeting on

Trends in Biotechnology: a Challenge for the Chemist

7 August 1995, 14.00–16.00 hours
University of Surrey, Guildford,
Lecture Theater Bldg: Theater M
Convenor H. G. Leuenberger
F. Hoffmann-La Roche Ltd, Basel.

Program

J. Kas, Institute of Chemical Technology, Prague: Bioanalytics
The state-of-the-art in the interdisciplinary field of bioanalytics will be presented. The broad analytical potential of modern enzymatic methods and immunological techniques will be discussed. Substantial progress has been made by combining biological elements (cells, enzymes, receptors, antibodies, etc.) with well established analytical systems (e.g. electrical/ electrochemical devices) leading to various types of highly specific and sensitive biosensors. Further, DNA amplification by PCR technology offers a unique tool for the accurate detection of DNA sequences and therewith for a broad scope of analytical applications.

H. Kölbl, Bayer AG, Leverkusen: Combinatorial Chemistry
Through new developments in biotechnology characterized by buzzwords such as 'Combinatorial Libraries' and 'Evolutionary Biotechnology' chemical synthesis is challenged with so far unseen requirements. The talk will discuss competing philosophies and strategies in chemistry and biotechnology.

J. Tramper, Agricultural University, Wageningen: When and how to use a biocatalyst for synthesis?
In this presentation, the following topics will be discussed:

- Chemical vs. biosynthesis, isolated enzymes vs. whole cells.
- Free vs. immobilized biocatalysts, aqueous vs. non-conventional media. Conventional vs. novel bioreactors.
- (Fed) Batch vs. continuous operation, segregation vs. integration.

Changes of Meeting Rooms

Organic Chemistry Division (III) Open Meeting on Monday 7 August, at 14.00–17.00 hours will take place in Lecture Theater (LT) F (not LT M).

The Table below lists a number of additional meetings for the General Assembly.

Committee on Chemistry and Industry(COCI) Proceedings of the 2nd IUPAC Workshop on Safety in Chemical Production, Yokohama, Japan, 31 May – 4 June 1993

The international Union of Pure and Applied Chemistry has perceived that the issue of safety in chemical production and the technologies for handling chemical substances is one of IUPAC's greatest challenges, recalling some of the catastrophic chemical accidents, and the recent interest in global environmental problems.

With this concern, IUPAC–COCI (Committee on Chemistry and Industry), held the 1st International Workshop in 1990 in Basel, Switzerland in cooperation

Subject	Date	Rooms	
Clinical Chemistry Division Committee	6 August 1995	14–17	[TB18]
	7 August 1995	9–12	[TB18]
Subcommittee on Transport Properties	7 August 1995	14–18	[5AA19] (OP/SP)
	8 August 1995	9–13	[3AZ18](OP/SP)
		14–18	
Destruction of Chemical Warfare Agents	5 August 1995	9–13	[Lakeside Rest AZ]
	6 August 1995	9–13	[TB18]
		14–17	[23AD21]
WP on Quality Systems in Clinical Laboratories	5 August 1995	9–13	[26 AA 19]
		14–18	[26 AA 19]
Destruction of Chemical Warfare Agents	7 August 1995	9–13	[Lakeside Rest AZ]

with Swiss chemical companies. Industrial, governmental, and academic experts on the safe production of chemicals from advanced and developing countries were invited to attend the workshop.

The United Nations Industrial Development Organization (UNIDO) assisted this Workshop by inviting participants from developing nations. The participants discussed the international efforts needed to allow the safe production of chemicals, and how best to protect the global environment, and in so doing recognizing the importance of this type of workshop.

Based on its initial success, IUPAC–COCI held the 2nd workshop on Safety and Chemical Production in Japan, where the chemical industry has accumulated extensive experience and expertise on safety in chemical production and have made extensive investments in facilities for environmental protection.

Representatives of IUPAC in Japan assisted in organizing this meeting which was held in Yokohama 31 May – 4 June 1993 in cooperation with Japanese chemical companies who believe that responsibility for safety and environmental protection must be part of their corporate policy.

The aim of the Workshop was to focus on the present status of safety and environmental protective measures for selected chemical processes. Knowing that for each specific process there were several solutions based upon the differing governmental regulations, and the varying educational or technical background of the workers, the goal here was to disclose to the participants the diverse facets of the current picture on safety and environmental protection in chemical production. Governmental experts, representatives from educational institutions, and industrialists had the opportunity to learn from the specific examples presented, and to select those innovations which could be implemented or might become applicable in their home countries.

The first day of the Workshop provided information of the safety management, education and training at chemical plants and universities. On the second day, evaluation of hazards and several engineering problems such as AI systems, fuzzy control systems and inspection standards, were introduced and debated. The third day's event was a factory tour with detailed case studies provided by the corporations operating in the Yokohama area. On the morning of the last day, panel discussions were held, some technological and political subjects such as safety science and technology, the proposal for the establishment of an international education center, and the future of IUPAC COCI Workshop were discussed. Finally in the afternoon of the last day the draft of 'Recommendations' was proposed and presented by the Organizing Committee and ratified by the conference.

Recommendations of the 2nd IUPAC–COCI Workshop on Safety in Chemical Production Yokohama, Japan

Rationale

The goal of the organizing committee was to offer an opportunity for leaders from academia, government and industry to:

(a) critically examine current practices;
(b) exchange ideas and experiences;
(c) discuss important issues with respect to safety and environmental protection.

The committee also recognized the importance of hands-on experience and extended these discussions outside the formal meeting into neighbouring plants.

Chemistry is the fundamental basis for all life. Chemistry and chemical technology are not only essential for the maintenance and improvement of every day life, but they are also vital for the continuation of technological advancement based upon progress in fundamental research. Risks associated with the production of chemicals have to be maintained at the lowest tolerable level in order to protect mankind, the global environment and to ensure sustainable development.

Adequate safety management of the whole product life cycle including research and development, production, transport, storage, consumption and final disposal is urgently required. Such management and stewardship is the common responsibility of academia, government, industry and consumers in both developed and developing countries.

The following recommendations have been put forward by the organizing committee of the 2nd IUPAC Workshop and ratified by the conference. It is expected that they will be transmitted by the participants to influential opinion makers world wide. They will also be distributed within IUPAC.

Measures for chemical safety and environmental protection in production and research

Appropriate measures for chemical safety in production and research may be described by a structure interconnecting the five following elements: chemicals, facilities, procedures, human factors and management.

Chemicals

Any person using chemicals in industrial and academic research organizations should foresee, and assess, all possible hazards including those which endanger mankind, the environment, and the production facilities. Appropriate measures should be taken to control all hazardous situations.

Facilities
All the facilities and apparatus for research, production, storage, loading/unloading, transportation, treatment, use and disposal should be designed and engineered to reduce the risks of chemicals and processes. Such facilities should be manufactured, constructed, operated, maintained and inspected with attention.

Procedures
The effective control of hazardous materials requires an ongoing commitment to the principles of process safety management. This was defined by the conference as the application of systems and controls (including programs, procedures, audits and evaluations) to a manufacturing or chemical process in a way that incidents arising from process hazards are prevented.

Human factors
The personnel should be educated and trained to recognize potential hazards, to follow operating manuals and to understand emergency procedures. The individuals must take responsibility for their own actions towards corporate goals. They should be motivated to propose 'bottom up' activities, and to show voluntary commitment towards furthering safety and environmental protection.

Management
Managers at all levels are responsible for the administration of chemicals and facilities. They should recognize the hazards of chemicals, characteristics of human behaviour, and be committed to the active implementation of integrated safety and environmental protection.

Cooperation for loss prevention and environmental protection

Cooperation between academia and industries
Academia has a vital role to play in partnership with industry. Course design, delivery and evaluation should best meet the needs of industry and embrace the existence of academic expertise in safety and environmental protection. Academia should also adopt appropriate safety and environmental protective measures within their own research domain.

Cooperation among industries
Industries should exchange data pertinent to safety and environmental protection. This information should include details (*inter alia*) of safety management policy, new safety technology and hazardous events. They should also cooperate to promote their principles of 'Responsible Care' towards their products over the whole life cycle. Such cooperation requires industries to provide appropriate information in an internationally accepted format.

Cooperation between industries and government
Government and industry should make concerted efforts to maintain a close relationship. This will enable all governments to produce appropriate legislative instruments for safety and environmental protection and to further ensure the exchange of information.

International cooperation
Developed and developing countries should cooperate to promote the exchange of information concerning safety management and environmental protection including details of hazardous events. International measures should be taken to promote appropriate training, e.g. by establishment of international training centres.

Committee on Chemistry and Industry(COCI) Minutes of the meeting held in Shanghai, China, 8 October 1994

The 17th annual meeting of COCI was in the city of Shanghai (People's Republic of China) on 8 October 1994.

The President thanked the Shanghai Petroleum Company for its invitation and for having organized the meeting on its premises thereby facilitating COCI members to visit the Jinshanwei industrial site after the meeting.

The President thanked Prof. Albert Fischli, former president of COCI, and now Vice-president of IUPAC, for attending the annual meeting. The President welcomed the participation of many delegates, including Dr Min Che Chon representing South Korea, Prof. Shatzmiller representing Israel, Dr Senti representing Switzerland and Mr Daniel Michalet (France) as Secretary of the COCI.

Company-associates status and outlook

Prof. Fischli spelt out the rules governing the contribution of company associates. Under the rules of IUPAC (see Blue Book, page 48), countries that pay more then 40 units, e.g. Japan and the United States, are entitled to two representatives. The same normally applied to regions which contribute more than 40 units; this is the case of the European Union.

There followed a discussion which revealed that engineering and production personnel were underrepresented on COCI and that countries that have two representatives should choose them so that they compliment one another in research, production and safety disciplines.

Moreover, action should be taken to elicit new members: It was decided to send the recently produced IUPAC leaflets to:

- the Chief Executive Officers of companies who are not yet members of COCI in the member countries of COCI;
- to Chief Executive Officers of countries not yet members of COCI;
- members are asked to send the list of the Chemical Companies of their countries for those who have not yet seen this list.

Retrospective of the past year

The main actions of the past year focused on: 'Chemistry for life'.

Many actions were undertaken in 1994 to promote chemistry and its public image as part of the celebrations for the 75th anniversary of the IUPAC. These celebrations vary greatly from country to country: e.g. lectures, poster competitions highlighting the 'chemistry for life' theme, magazines and books, TV programmes.

Many Nobel prize winners took part in these events:

- in Winnipeg, Canada: on 29 May the Symposium 'Chemistry for Life' assembled four Nobel prize winners: Gerhard Herzberg, John Polaniy, Rudy Marcus and Michael Smith;
- In Washington (USA): for the 75th anniversary of the IUPAC: Glenn Seaborg;
- in Brussels (Belgium) for the 29 May celebrations to mark the 75th anniversary of the IUPAC, Jean-Marie Lehn and Lord Porter;
- in Taipei (Taiwan), for the 12th October celebrations to mark the 75th anniversary of the IUPAC, Yuan T. Lee.

COCI greatly appreciated the production of a large collection of slides designed to show the chemical industry in an attractive light. This contribution by Belgium was made possible due to the generosity of the Agfa Gavaert company which COCI would like to thank. These slides are currently available in Flemish and French and it might be useful to translate them into different languages.

Representatives from those countries interested can obtain these slides by writing to:

Dr F. Claes, Agfa-Gevaert, Septestraat, B-2640 Antwerpen-Morstel, Belgium

Regional activities

In Europe, the 75th anniversary of IUPAC was jointly celebrated on 26 May by the CEFIC and COCI, on 26 May with the participation of two Nobel prize winners and may dignitaries.

In Asia, the regional committee met on 12 October in Taipei (Taiwan) and was attended by Prof. Albert Fischli.

Collaboration with UNESCO–UNIDO

The IUPAC–UNESCO–UNIDO Fellowship Program initiated by COCI is now underway. It is the only program in existence between IUPAC and UNESCO-UNIDO with whom it is very favourable received.

An initial group of five company safety officials from developing countries were able to stay in major European companies between December 1993 and the summer of 1994.

It is important to continue this experience and COCI asks all its members to urge their national companies to host experienced safety officials (not beginners) on 2–3-week placements.

'Chemistry for the 21st century' monographs

The Editorial Board responsible for producing these monographs seeks the help of a representative from industry.

COCI and the chlorine ban

The Chairman raised important issues such as the ozone hole and the toxicity attributed to organic chlorine molecules, which in certain cases threaten whole sectors of the chemical industry. COCI must turn its attention to these issues.

The Chairman informed members of the project of Prof. Alan Bard, president of IUPAC, to involve the Union in the question of the chlorine ban. The aim is that the IUPAC shortly publishes an authoritative scientific report on all aspects of the question so that the public authorities draw on this document in their discussions with industrialists and environmentalists.

Outlook to the 3rd IUPAC workshop on safety in chemicals production

The 3rd IUPAC Symposium on Safety in Chemical Production will be held in April 1996 in New York at the United Nations.

The symposium enjoys the support of the ACS and the CMA. It could be divided into three parts:

- Communication;
- Visit to an industrial site;
- Resolutions.

It is also proposed to make copies of the book of the Basel symposium and to offer them to chemical engineering faculties.

Discussions about possible COCI contributions beyond 1995

The President set out the proposals of COCI members who could not attend the Shanghai meeting. The following themes were proposed:

1 Outline themes concerning the image of chemistry and safety in production.
2 New topics proposed: the environment, the problem of water, the search for radically different processes producing practically no effluents, catalysis, the input of research for safety, engineering geared to the automation of safety and the gap between education and safety.

The water situation

Prof. De Bievre, who wished to enter this topic on the agendas of COCI meetings, highlighted the importance of having comparable and reliable assays so that regulations could be laid down (e.g. drinking water, irrigation water).

Taking as an example the results of lead measurement in different specialized laboratories, he showed that no regulation can be laid down at present for want of a reliable and reproducible method.

IUPAC–COCI leaflets

Prof. Fischli has launched a recruitment Campaign to obtain more numerous and more committed company memberships. Taking this opportunity, it was decided to send leaflets to all CEOs. COCI members are requested to supply the names of CEOs an their addresses in non-member countries such as Australia, Austria, the Czech Republic, Egypt, Eire, Hungary and the Republic of Slovakia.

The next meeting of COCI will be at the General assembly, Guildford (UK), on 7–8 August 1995.

Daniel Michelet (Secretary)

Commission on Nomenclature of Organic chemistry (III.1)

Minutes of the meeting held in Balatonfüred, Hungary on 4–8 September 1994.

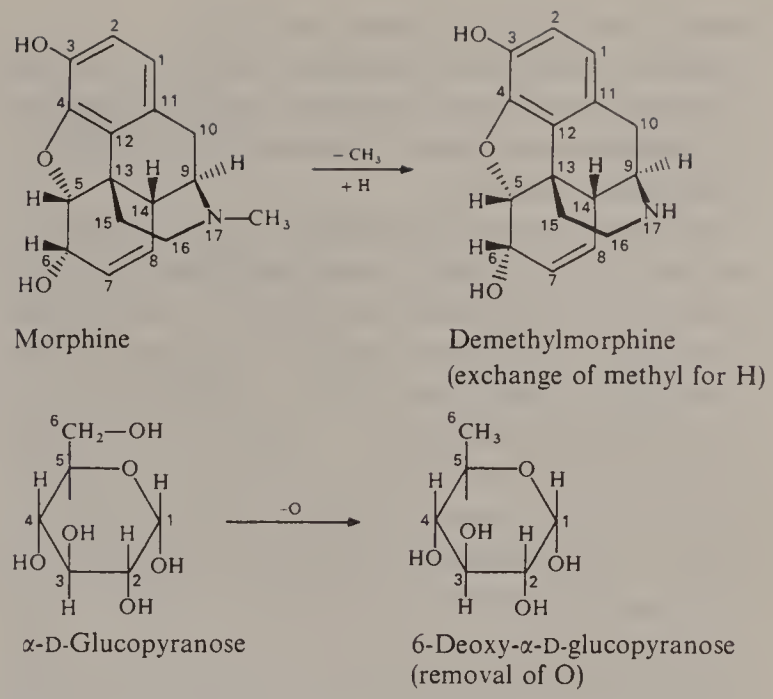
The principal points made in the discussions are summarized for each project (document).

Priorities among classes of compounds

There was a general discussion on 'zwitterions', which included a suggestion that the term be dropped. Question: Why is peroxide senior to oxide while amide is senior to hydrazide? Ylidene amines should be named as imines.

Priorities among suffixes

Ylides would be named normally by substitutive methods. Retain 'pyridine *N*-oxide' rather than *N-oxidopyridylium*. The distinction between Group I (cumulative) and Group II (solitary) suffixes is very useful. Tellurocarboxylic acids will be included. Formic and



Naming, by use of a prefix.

oxalic acids are formally carboxylic acids. Boronic, borinic, and chloronic acids must not be forgotten.

Ring and chain priorities

No document was ready for distribution to the commission. The discussion focused on issues of centrality directing decision on priority. A phane approach seems to relieve the priority question with some multi-ring/multi-chain structures. R.B. de Alencastro distributed a draft statement with a simple rule for deciding priority: If number of rings is odd (central) ring has priority for parent; if even (central) chain has priority. Members of the commission asked for simple rules that will be easy to teach.

Order of operations

W. H. Powell presented two documents, which had been distributed to attendees before the meeting (1) A comparison of Nondetachable Hydro Prefixes, Added Hydrogen (CAS) and Indicated Hydrogen (Beilstein) in Expressing Substitutive Suffixes and (2) Order of Citation of Name Components in a Systematic Structural Nomenclature for Organic Compounds. He explained that the first document did not present new nomenclature, rather it made a comparison and explanation of three different methods. O. Weissbach expressed some objections to the text about the Beilstein method. W. A. Powell said that he is willing to consider Weissbach's comments, but he pointed out that the document was approved by CNOC last year (except for the Introduction). The matter was referred to the P (d) Subgroup. The last two suffixes still need attention. Calling -ene and -yne flexional-endings rather than suffixes would eliminate some of the problem of cumulative suffixes. Cyclo was discussed as to its position in the citation order.

Basis Terminology of Stereochemistry

G. Moss reported that virtually all workers in the field are happy with what is in the document. No fundamental disagreements persist. However, the definition of *meso* needs attention.

President Oki suggested that documents now available only as *Pure & Appl. Chem.* reprints might be combined as a book jointly published by two or more commissions. The commission discussed the on-line accessibility of these documents. G. Moss volunteered to put *Basic Terminology* ... on-line and will inform IUPAC officials of what is being done so that objections, if any, can be registered. He then summarized a short paper on stereochemistry of organic compounds having a geometry other than tetrahedral; namely, trigonal bypyramid, square pyramid, and octahedron. (Other geometries in the Red Book do not involve compounds named by organic nomenclature.). Question: How does one include stereochemical descriptors for different kinds of chirality in the same molecule? The matter was referred to the P(e) Sub-group.

Computer-adapted nomenclature

J. Wisniewski reported that AUTONOM is selling well (about 500 copies) and that different versions are available. The latest version costs USD1150 for individual users. The success rate is 85%, the 15% failure rate means that the AUTONOM program simply cannot generate a name for a structure presented, not that it generates an incorrect name. AUTONOM always gives the same, single name for a structure; that is its great strength. Stereochemistry is not yet included, but that version will probably be ready in 18 months. The program now handles charges. Beginning next year the Aldrich catalog will include the AUTONOM name for every entry. Only IUPAC rules are used. AUTONOM will be modified from time to time to try to incorporate preferred names as they are established by CNOC.

R. J. Hwu commented on the success of AUTONOM with its students, but he does find the multiple brackets troublesome. E. W. Godly agreed with J. Wisniewski that 'in house' rules are necessary for consistency in names for commerce; he emphasised a difference in emphasis on an archival name and on a practical name. J. Wisniewski invited E-mail communication from CNOC participants about AUTONOM.

P. M. Giles was invited by the chairman to speak about CAS efforts in this area. No commercial program has been produced yet. There has been extensive development of an internal program. CAS intends to rename the entire data base of 13 million compounds by its program when one is complete. Editing of the data base will take place concurrently. The developing program is not user-friendly in its present form, but the version that gets commercialized is likely to be so. B. Herold spoke in favour of user friendly names; simple names are generated by complex rules.

Natural products and related compounds

P. M. Giles reported that he has received some comments on the Revised Section F document (May 1994), and he invited CNOC participants to submit further comments. The working party will consider the comments, which so far have not called for any substantive revision. A footnote about objection to -ine ending for unknown isolates is to be added. The term 'atomic connectors' was discussed. Is expansion of the vocabulary required for clarity (e.g. homoatomic, polyatomic)? Alternative terms 'chain connectors', 'connecting chain' and 'connecting bond' with terms italicized in text, were suggested.

Hydrogenation of parent hybrides

B. J. Herold presented a summary of different definitions of 'parent hybride', raising a number of questions which need to be settled to guide further work in this field. E. W. Godly agreed that the loose approach of the past must be superseded by firm decision on dihydro/dehydro usage. Herold summarized a possible mathematical rule for determining a dividing line between mancude and cyloalkane parents being modified. Should annulenes be treated the same as benzene? Monocyclic mancudes are treated differently from polycyclic mancudes (benzene vs. napthalene or anthracene for example).

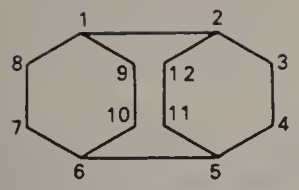
New principles

Fullerene nomenclature

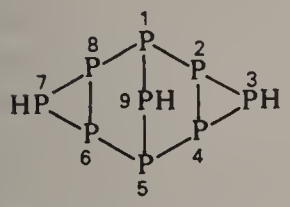
A. D. McNaught referred to the IUPAC special group on fullerent nomenclature: members are workers in a rapidly expanding field, with minor representation from CNIC and CNOC. A report was presented to IDCNS accompanied by a request for a shortened review and the opinion that no public review was needed. The approach in the IUPAC draft diverged substantially from the CAS approach, which had been in use for some time, because of the immediate need for indexing. Publication of such divergent recommendations was viewed as unwise, and the two groups are now trying to get together. The major priority is establishing the numbering system.

The chairman appealed to the fullerene committee to be strict when using the organic rules; e.g. fullerane for C_{60} H_{60} is not the conventional use of -ane ending. If new compounds do not fit definitions that affect nomenclature, new nomenclature will be needed.

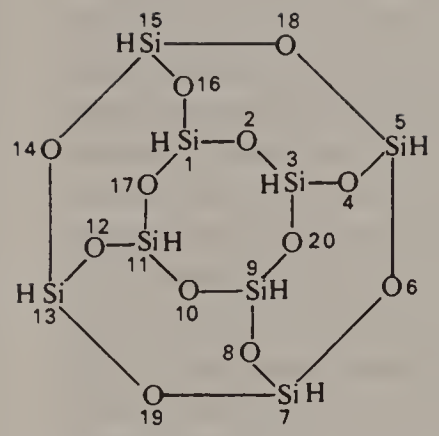
Should the CAS method be included if the IUPAC recommendation is different? If there is no common ground, the IUPAC will have no recommendation as such and a description of the two approaches should be presented. The consensus was that whether IUPAC makes a firm recommendation or not, comparison of



Tricyclo[4.2.2.2^{2,5}]dodecane



Tetracyclo[3.3.1.0^{2,4}.0^{6,8}]nonaphosphane



Pentacyclo[9.5.1.1^{3,9}.1^{5,15}.1^{7,13}]octasiloxane

Prefixes such as *1Si-* and *1P-* are used in polycyclic systems of alternating skeletal atoms when it is necessary to indicate the atom at the bridgehead that is to have the locant '1'.

the two approaches should be made in a document, because that will be useful to workers for 'translating' different publications.

Phane nomenclature

O. Weissbach presented a document and identified four kinds of criticisms. (1) discrepancies in the extension of von Bayer nomenclature to include pairs of bridgehead atoms linked by more than three independent bridges; (2) doubts about the merit of alphabetical order for replacement ring prefixes and/ or of the use of English prefix order for numbering; (3) unintended extension of the Part I paper to details to be covered in future documents, and (4) need for clarification and difficulty of understanding. Several CNOC participants said that no meaningful seniority order is in place as a useful alternative to alphabetical order.

Educational publications

The suggestion made last year that the *Guide* be distributed to textbook publishers was not supported because of the cost. The committee will further examine the issue. CNOC participants made several comments about the poor publicity and distribution of IUPAC documents.

H. A. Favre is the Organic Division representative for the *Manual*, which is aimed at students and teachers. A draft of 80 pages of nomenclature had to be reduced to about 40 pages for the *Manual*, but the authors thought that an expanded version (about 160 pages) integrating organic, inorganic, polymer, and biochemical nomenclature would be useful. If these two documents materialize, they will be good publicity for IUPAC nomenclature activities early in teaching. They will also de-emphasize separateness of inorganic and organic nomenclature. The probable date for presentation of the final document for the *Manual* is August 1995 at the Guildford meeting.

Organometallic compounds

E. W. Godly reported that the joint meeting on 3 September 1994, was attended by nearly all CNIC and CNOC committee members. CNIC is particularly interested in publication of a book on organometallic nomenclature, one that can stand alone without necessary reference to Red Book, Blue Book, or *Guide*. Preparation of the book needs input on main-group elements from CNOC. Ferrocene needs to be ranked as a parent hydride. CNIC is considering CNOCs order of anions for application to organometallics; this approach will better signify the actual coordinating site.

Reports of Convenors Following Meetings of Sub-group

Glossary of Class Names

D. Travernier reported that the public review of this document in 1993 produced favourable reaction and some especially helpful comments from reviewers. Dr Neumüller, editor of *Rompff"s Chemie Lexicon* was particularly cited. A revised version of the *Glossary*, incorporating suggestions of reviewers, was circulated to sub-group members before the 1994 meeting, and the entire 77-page document was carefully reviewed at this meeting. Two entries merit mention: The *Guide* definition of 'annulenes' (rings with at least seven members) will be cited, followed by a statement that, in the primary literature, rings with fewer members are commonly subsumed; and 'organyl' includes acyl (in accord with use by the majority of senior authors of the primary literature). The manuscript is in final form and will go to Commission III.2, M. Oke, and IDCNS.

Fullerenes

A. D. McNaught reported that *ad hoc* working party had made much progress in its 3-hour meeting, and he commended R. Taylor and E.W. Godly for producing a working document that enabled the working party to be so fruitful. Items agreed upon by the working party included: (1) The narrow definition of fullerenes (five- and six-membered rings) will be retained, and analogs will be called quasi-fullerenes. (2) The naming style of the Taylor–Godly document for fullerenes, without specifying ring size, will be used; for quasi-fullerenes, ring size could be specified in parenthesis in front of the parent name. (3) Both the Taylor and CAS methods of numbering should be included in IUPAC fullerene document without specifying an IUPAC preference. The Taylor approach can be regarded as analogous to 'natural product' numbering in the Section F document, and the CAS approach as a more systematic alternative. Agreement on numbering of systems other than C_{60} and C_{70} is to be considered. (4) Stereochemical clarifications included adding *C or A* enantiomer designations to all diagrams of parent fullerenes. (5) Hydro prefixes will follow the non-detachable principle. Examples of simple derivatives will include same CAS names (and numbering), in particular a name with CAS 'added' hydrogen. A fullerene parent will not be regarded as a center of coordination. Examples of bridging and fusion methods will be included, but these methods will be adapted to leave the numbering of the fullerene nucleus undisturbed. 'Homo' is to be used as in Section F. The radical anion formed by electron addition to fullerene is to be named fullenelide. The text and example(s) will be revised to present compounds in which fullerenes are ligands. R. Taylor has agreed to revise the document to incorporate these agreements.

Cyclic systems

A. D. McNaught reported several decisions pertaining mainly to spiro structures: (1) Replacement and multiple bond operators will be placed outside the parent names of the 'spirobi' types, except for other spiro combinations with different components. (2) Non-standard valency at a spiro atom will be symbolized separately from the spiro position locants (e.g. $2\lambda^6$–2,2′,2′′ – spiroter …). (3) The numerical terms in dispiro, trispiro, etc. shall refer to the number of rings. (4) The meaning of 'spiro' will be clearly explained by a sentence added to the document. (5) 'Circular' dispiro examples and their implications for phane nomenclature will be considered. (6) Next drafts of the spiro and von Baeyer documents are to be circulated in the next year. (7) A proposed compendium of ring nomenclature, while probably used to specialists, would have doubtful marketability, and the usual IUPAC publication channels might be inappropriate.

James G. Trajnham (Secretary)

Macromolecular Division

Minutes of the Meeting of the Working Party on Recycling Polymers, Arlington, Virginia, USA, on 18–20 July 1994.

Members presented brief reports on the topics they has researched during the previous year. Dr Mader stated that the world-wide consumption of polymers is *c.* 100 million tons/year, of which Europe consumes 30 million. He believes that packaging is the most important consumer followed by automotive applications. Polymers are tailor-made for each application; thus there is a multiplicity of grades which render polymers so useful to society. We should devise concepts for waste management with optimization of resources and minimization of energy usage. On this basis, polymers may be viewed favourably as part of sustainable development. This could be made clear if a 'polymer cycle' could be devised, similar to the C and N cycles. However, the loop would not be closed since there would always be losses due to degradation of polymers. Plastics can be considered to be an intermediate stage of storage for the energy in crude oil. Thus, attention should be paid to resource recovery rather than disposal of waste.

Dr Brandrup discussed mechanical recycling, and pointed out that except for PET bottles, recycling of plastics is not economically favourable. Most packaging weighs less than 10 g, so collection entails large energy costs.

Dr Brandrup pointed out that feedstock recycling (cost *c.* DEM650/ton) is the best solution for mixed, contaminated polymers if incineration with energy recovery (cost *c.* DEM200–300/ton) is not possible. The waste material for each chemical process needs to meet certain specifications. About 10 p.p.m. Cl is present even if there is no PVC in the waste. Waste can be subjected to a thermal treatment ('hot box') to decrease or eliminate halogens and to depolymerize polymers. The feedstock may be suitable for syngas production, but unsuitable for the oxo reaction because it contaminates Pd catalysts.

Prof. Akehata reported that, in Japan, plastics manufacturers and MITI favour energy recovery through incineration instead of land-filling. Combustion can be made very efficient and produce low emissions. Pyrolysis is well developed both for post-consumer and industrial waste plastics. Studies in Germany have shown that increasing the plastic content of incinerated waste does not increase the levels of dioxin, carbon monoxide, etc., and that all German and US regulations can be met with respect to emissions.

Dr Schnecko reported that reclaim is not used much, except in Japan, because the process is dirty. Retreading of large tyres is used to diminish the amount of waste; for example an aeroplane tyre can be retreaded

about ten times. The EU is now working on recommendations for scrap tyres. An experimental method is microbiological degradation of vulcanized rubber, which cuts the sulfur bridges and makes the waste processible. Cryogenic crumbling gives smooth particles, but with decreased adhesion to other surfaces. The use of tyre crumb in asphalt road surfaces is being projected in the US.

Prof. Marchessault reported that biodegradable polymers will not solve the problem but could contribute to a solution. The topic is very timely, and part of the 'green revolution'. He described advances in the UK, US, Japan, and Sweden. Biodegradable polyesters can be made as plastics, elastomers, and medical biomaterials. Their price could fall sharply if they can be produced by agriculture rather than biotechnology. An important issue is whether biodegradable polymers would interfere with the recycling of nonbiodegradable polymers. ASTM is developing a standard test. For the foreseeable future, biodegradable polymers will only fill a market niche.

Reporting on Germany, Prof. Heitz said that polymer waste has been reduced by decreasing the weight of packaging, e.g. for yoghurt. Packaging used in transport and as outer packaging is collected separately from other waste. Retail packaging is placed by the consumer in a 'yellow bag;' this procedure is widely accepted. Quotas have been placed on manufacturers that require 80% recycling in 1995 (equivalent to 64% of consumed plastics), but the capacity for disposal of mixed plastics is insufficient. Nevertheless, some large plants exist: VEBA and Hydrierwerke plants have capacities of 120 000 and 100 000 tons/year, respectively, for hydrogenolytic degradation to an oil residue, and BASF can treat 300 000 tons/year by thermal cracking. The EU parliament has passed laws, still to be ratified by the Council of Minister, that will require recycling of a minimum of 15% for each material in the waste and 25% min. and 45% max. recycling for all materials.

Prof. O'Donnell stated that in Australia, recyclable consumer waste is divided into two containers, one for paper and the other for glass, metals, and polymers. Polymer waste represents *c.* 5% by weight of the total, of which bags are 13%. He believes that our report will be useful as an educational tool.

Dr Bikales discussed his progress in terminology and nomenclature, and there was a lively discussion of the terms 'scrap' and 'waste'.

The Working Party then recommended that the 1997 IUPAC meeting in Prague select as its themes: Strategies for recycling; New Processes and new concept; and Properties and uses. It agreed to help in shaping the program, if requested.

The next meeting of the Working Party will be held at the IUPAC General Assembly in Guildford, UK, preferably on 3–4 August 1995.

Norbert M. Bikales (Chairman)

IUPAC colleagues deceased

USA Mr P. M. Arnold (28 October 1994) – Bureau (1969–75), Executive Committee (1971–75), Finance Committee (1963–71).

USA Prof. C. Ponnamperuma (23 December 1994) – CHEMRAWN Committee (1988–94).

Periodic Minimal Surfaces in Chemistry

The last few years have seen something of a revolution in structural crystallography. First, the rigid concept of the perfect crystal has been relaxed to embrace more general structures such as quasi-crystals. A diffraction pattern would previously have been seen as a collection of well-defined sharp Bragg peaks observed against scattering angle with a flat background between each Bragg peak. In a powder diffraction pattern, for example, the angles at which the peaks appear can be analyzed to give information on the nature, symmetry, of the unit cell and the intensities of the Bragg Peaks may be analyzed to give the orientation of the molecules, which contain the scattering atoms, within the unit cell. An experimenter would have been looking for very sharp diffraction lines measured against a flat background. In such an experiment, the scatterers would have been well localized, indeed, frozen within the solid and information about their relative positions could be inferred from the diffractogram. The final experimentally derived information, for example bond lengths and intermolecular distances, being determined with very high precision (0.01 nm).

Today, with more sensitive diffractometers and sophisticated computer software one may also use neutron and X-ray diffraction to probe the motion of the molecules in the unit cell. What would previously have been seen as unwanted small intensity shoulders on each side of a Bragg peak, or broad undulations of the background level, may now yield dynamic information on the motion of the scattering particles in the solid-state. Previously, these shoulders would have been an inconvenience which reduced the quality of the statis-

Figure 1 A soap film showing the curved surfaces which may be represented by minimal energy surfaces.

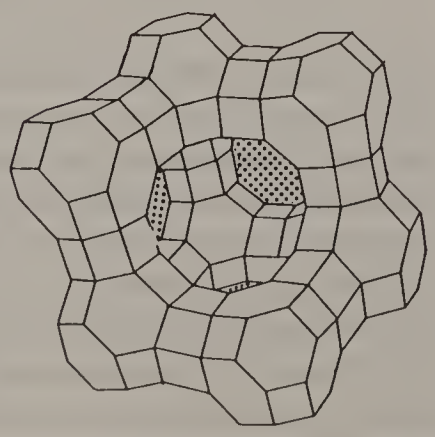
tics (if the observed line is very broad then its center point is not well determined), now such shoulders on Bragg peaks tell us how, for example, rapidly a molecule is rotating in the solid.

The ability to interpret the scattering from non-perfect structures, for example, a benzene ring rotating about its C_6 axis within the solid [as happens in solid benzene at temperatures between 150 K and the melting point of solid benzene at 278 K where the frequency of rotational motion follows an Arrhenius behaviour [$\nu = \nu_0(77\ cm^{-1})\exp(-12.5\ kJ\ mole^{-1}/RT)$], has come about through advances in our ideas of the application of three dimensional differential geometry to solid-state structures. The decisive step in this direction has been the use of curved surfaces in describing a variety of seeming unrelated structures. To understand the structures of complicated natural solids, or indeed of interfaces, it is no longer necessary to think of the scattering atoms as being frozen on planes within a solid.

The essence of the concept of a minimum surface is as follows. When a wire frame is dipped into soapy water, a thin film is formed (see Fig. 1). Surface tension, which is proportional to the surface area, minimizes the energy of the film. Consequently, the film has the smallest area consistent with the shape of the frame and with the requirement that the *mean curvature* of the film be zero at every point.

At any point P on a surface there exists a uniquely defined vector normal to the surface, a plane containing this vector intersects the surface, forming a plane curve. The curvature of this plane at point P is known as the normal curvature of the surface in the tangent direction of the curve. The maximum and minimum values of the normal curvature are the 'principal curvatures', k_1 and k_2, respectively, and tangent directions of the corresponding curves are 'principal directions'. The principal directions are normal to each other. The mean curvature of the surface at point P is defined as, $H = (k_1 + k_2)/2$. A minimum surface is a surface for which curvature is zero at all points. For many points $k_1 = -k_2 \neq 0$. Exceptionally, there are points with $k_1 = k_2 = 0$, known as 'flat points'.

If a minimum surface has space group symmetry, it is periodic in three independent directions; such surfaces are known as triply periodic minimal surfaces (TPMS), and are of special interest because they occur in a variety of naturally occurring structures. For example, the interface between single calcite crystals and the amorphous organic matter in the skeletal element in sea urchins can be described by the P minimal surface. That is, the experimentally observed three-dimensional molecular structure of the inorganic-organic interface in the skeleton of a sea urchin has the same symmetry properties as, is like, a particular well-known three dimensional mathematical function. Likewise, the



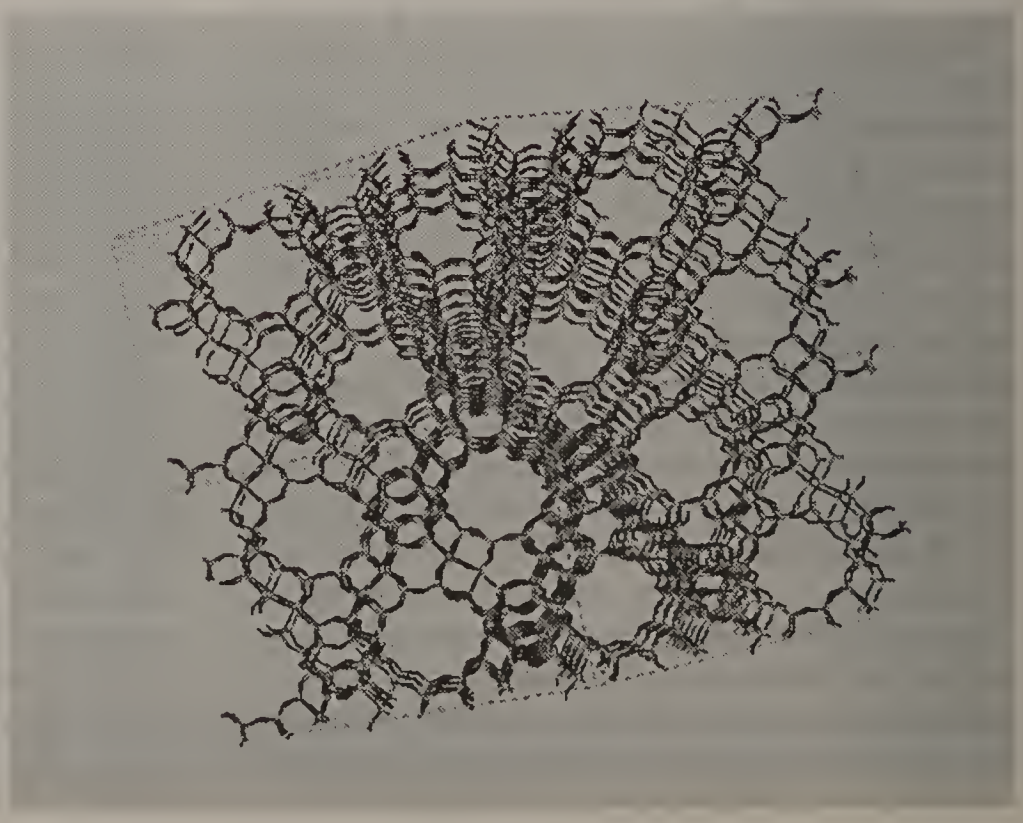


Figure 2 Faceted schematic representation of the structure of zeolite Y (above). The interlocking channels which characterize these open solids is more clearly seen in the image on the right, in which the individual chemical bonds are represented.

bicontinuous structures of liquid mixtures of water and organics, such as liquid crystals, are also minimal surfaces (the F minimal surface well represents the structure of a particular mixture of glyceryl mono-oleate and water) as are numerous zeolites. A zeolite is an open solid containing wide cross-linked channels through which small molecules may diffuse. They are exceptional catalysts. Figure 2 shows the structure of a particular zeolite, and the criss-crossing network of open channels is clearly seen. Many zeolites are naturally occurring, however, they may also be synthesized with variable structure.

It is the study of such microporous silica materials, synthesized in water-surfactant systems, which has brought the study of minimal surfaces to the forefront of structural chemistry. These solids, the structure of which mimic the liquid-liquid minimal surface, have drastically expanded the range of crystallographically defined pore sizes from the micropore (< 1.3 nm diameter) to the mesopore (2.0–10.0 nm diameter) regime. The synthesis of such microporous silica materials uses ordered arrays of surfactant molecules as a template for the three-dimensional polymerization of the silicates. Consequently, the final structure of the zeolite mirrors the interface between the different phases of the water-surfactant system.

It has been found, for example, that the cubic mesophase of these silicates is the same as the phase found in the water–cetyltrimethylammonium bromide system. The mid plane of the silicate wall lies on the gyroid G minimal surface. Such a structure may be viewed as a single infinite silicate sheet which separates the surfactant species into two equal and disconnected volumes. It is clearly advantages for the silicate wall to occupy a periodic minimal surface, because it can then maximize the wall thickness for a given surfactant/SiO_2 volume fraction.

Such investigations throw light on the mechanism of synthesis of these extremely important industrial catalysts, which are at present prepared mostly by trial-and-error methods.

Figure 3 represents a generated minimal surface. This structure is a representation of the solution of a particular set of mathematical equations. The similarity between this theoretical structure and the experimentally observed structure of the zeolite in Fig. 2 is clearly seen.

A periodic minimal surface must be examined in both a mathematical and a physical sense. They offer a unique way of expressing collective laws and strategies for understanding the larger correlations between related structures with potential for applications in molecular and materials design. Once the details of the parameters of a surface are known it is likely that one would be able to describe, quantify and predict transformation pathways in regular structures, such as solid-

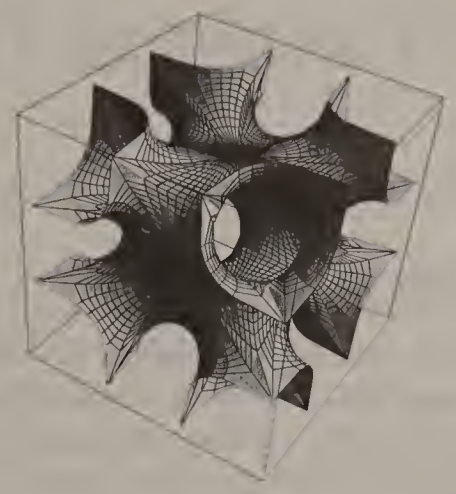


Figure 3 A generated minimal surface. This structure is a representation of the solution of a particular set of mathematical equations. The similarity between this theoretical structure and the experimentally observed structure of the zeolite in Fig. 2 is clearly seen.

state phase transitions in silicates and in water–oil–surfactant systems.

The coordinates of points lying on minimal surfaces are described in terms of integrals involving the *Weierstrass* function of the form

$$R(\tau) = 1/\sqrt{(\tau^8 + 2\tau^6\mu + \lambda\tau^4 + 2\tau^2\mu + 1)},$$

where μ and λ are parameters which fully describe the surface. It was thought that integration of the *Weierstrass* function could not be performed analytically. Numerical methods would have introduced approximations. However, Cvijovic and Klinowski (Department of Physical Chemistry, Cambridge, UK) have recently demonstrated that these *Weierstrass* integrals may be expressed as standard functions and they give explicit general equations for the coordinates (Cvijovic and Klinowski *Journal de Physique I (France)* **2**, 137, 2191, 2207 (1992); **3**, 909 (1993)). Thereby obviating the need for numerical integration. Indeed, the well known properties of the standard functions appearing in the solution provide new insights into the features of minimal surfaces and permit their systematic calculation.

The application of minimal surfaces to the physical world, in terms of describing in a relatively simple mathematical manner the structure of complex inorganic/organic materials, has so far been descriptive, rather than quantitative. The reason for this is that it was previously believed that the parameters of minimal surfaces could not be calculated analytically, while numerical calculations were inaccurate and consumed large amounts of computer time. However, it has recently been shown that it is possible to derive explicitly analytical general expressions for the parameters of TPMS and this has lead to the discovery of important new properties. The calculations can readily be undertaken on a personal work-station using a software packages such as Mathematica or Matlab.

Provisional Recommendations

IUPAC seeks you comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most up-to-date list of the national/regional centers appeared in *Chem. Intl.* **14**, 25 (1992) and in the latest *IUPAC Handbook (1994–1995)* published by Blackwell Science, 1994.

Recommendations for Nomenclature of Ion-Selective Electrodes (IUPAC Recommendations 1994)

The rapid growth of interest in the field of ion-selective electrodes, within the larger field of electrochemical sensors based on potentiometric, amperometric, and conductometric principles, makes it desirable to achieve an improved standardization of nomenclature in this area. The previous document, IUPAC Recommendations (*Pure Appl. Chem.* **48**, 127–132 (1976)) has been corrected using recent experimental and theoretical results. This present report does not, however, define or recommend activity standards or calibration procedures using activity standards.

This report was prepared for publication by Richard P. Buck and Ernö Linder, Department of Chemistry, University of North Carolina, Chapel Hill, NC 27599–3290, USA, who are members of the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The details are published in Pure & Appl. Chem. ***66**, 2527–2536 (1994).*

Nomenclature of Carbohydrates (IUPAC Recommendations 1994)

The earliest attempts at naming sugars was to give the molecule a name derived from the naturally occurring material from which the sugar was extracted – *nomen est numen*, to name is to know. For example, in the early nineteenth century, the name 'grape sugar', Traubenzucker, was used for glucose and 'cane sugar', Rohrzucker, for saccharose (sucrose was used as a name much later). The name 'glucose' was first used in 1838. Kekulé in 1866 was the first to attempt a system of nomenclature based on properties of the individual sugars. For example, he proposed the name 'dextrose' because glucose is dextrorotatory, and the laevorotatory fruit sugar, Fruchtzucker or fructose, was for some time called 'laevulose' (levulose in the United States).

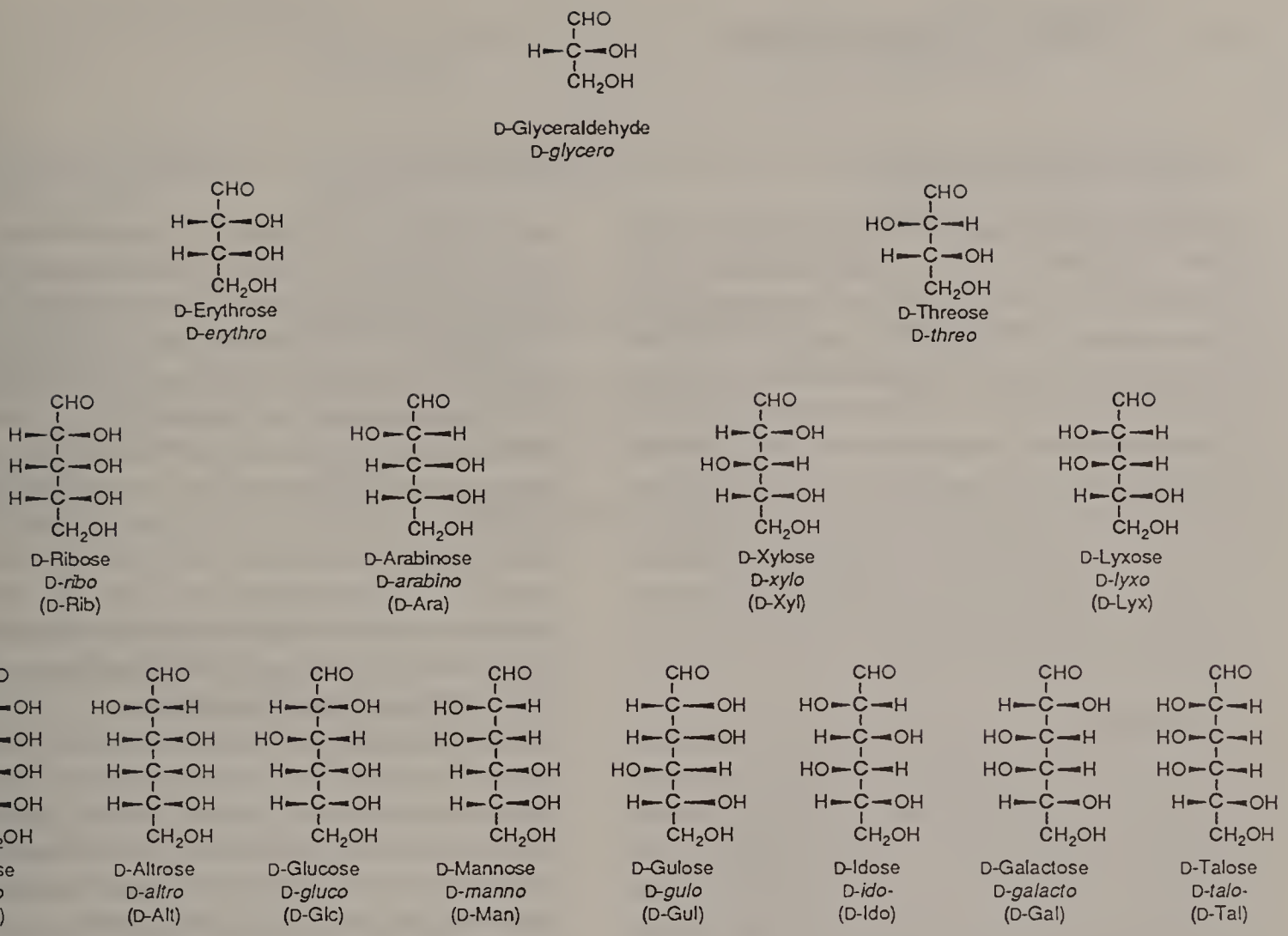
The word 'carbohydrate' comes from the French *hydrate de carbone* (when these substances were heated, it was observed that water was expelled and a carbon residue remained – resulting in a derived empirical formula of $C_n(H_2O)_n$), it was originally applied to monosaccharides only. Some consensus with regard to nomenclature of sugars was reached early on with the adoption of the ending '-ose', which combined with the French word for a cell, *cellule*, gives us 'cellulose'.

Emil Fischer began his studies of carbohydrates in 1880. Within ten years, he had assigned the relative configuration of most known sugars in addition to having synthesized many sugars. Fischer laid the foundations of the system of nomenclature still in use today. This system is based on the terms triose, tetrose, pentose and hexose. He endorsed Armstrong's proposal to classify sugars into aldoses and ketoses, and proposed the name fructose for laevulose, because he found that the sign of optical rotation was not a suitable criterion for nomenclature.

The introduction by van't Hoff and Le Bel of stereochemistry had a major impact on carbohydrate chemistry because it allowed one to explain isomerism. Fischer introduced the classical projection formulae for sugars, with a standard orientation – carbon chain vertical with carbonyl group at the top. He assigned to dextrorotary glucose the projection with the OH group at C-5 pointing to the right, however, it was in 1951 that he was shown, fortuitously, to be correct.

Rosanoff in 1906 selected the enantiomeric glyceraldehydes as points of reference, any sugar derivable by chain lengthening from what is now known as D-glyceraldehyde belongs to the D-series. This is a convention still in use.

The generic term carbohydrate includes monosaccharides, oligosaccharides and polysaccharides, as well as substances derived from monosaccharides by reduction of the carbonyl group (alditols), by oxidation of one or more terminal groups to carboxylic acids, or by replacement of one or more hydroxyl group(s) by a



Trivial names (with recommended three-letter abbreviations in parenthesis) and structures, in the acyclic aldehydic form, of the aldoses with three to six carbon atoms. Only the D-forms are shown, the L- forms are the mirror images.

hydrogen atom, amino group, a thiol group or similar heteroatom group or groups. It also includes derivatives of these compounds. The term 'sugar' is frequently applied to monosaccharides and lower oligosaccharides. It is of interest to note that 3% of the compounds listed by Chemical Abstracts Service, i.e. more that 360 000 molecules, are named by the methods of carbohydrate nomenclature.

These current Recommendations expand and replace the Tentative Rules for Carbohydrate Nomenclature jointly issued in 1969 by the IUPAC Commission on the Nomenclature of Organic Chemistry and the IUB–IUPAC Commission on Biochemical Nomenclature. The present Recommendations deal with the acyclic and cyclic forms of monosaccharides and their simple derivatives, as well as the nomenclature of oligosaccharides and polysaccharides. They incorporate material from later documents on conformational nomenclature, branched-chain derivatives and unsaturated monosaccharides. There are new sections on substituted monosaccharides (replacement of H or OH and the stereochemical consequences); monosaccharides as substituent groups; carbohydrate radicals; anions and cations; structures with ring oxygen replaced by other elements; and structures containing additional rings. An Appendix of trivial names with their systematic equivalents is included. They are additional to the Definitive Rules for the Nomenclature of Organic Chemistry, and are intended to govern those aspects of the nomenclature of carbohydrates not covered by those definitive rules.

Comments on these recommendations are welcome and should be sent by October 1st 1995 to:

Dr A. D. McNaught, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK, Tel.: (44) 1223 420066, Fax: (44) 1223 420247, E-mail: ADM@RSC.ORG

Cyclomaltohexaose (α-cyclodextrin, α-CD).

PAC Review

Pure and Applied Chemistry (*PAC*) is the official journal of IUPAC. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in *PAC* are published in *Chem. Intl.* in the section Recent Reports. In this section we take a brief look at the symposia and lectures published in recent issues of *PAC*.

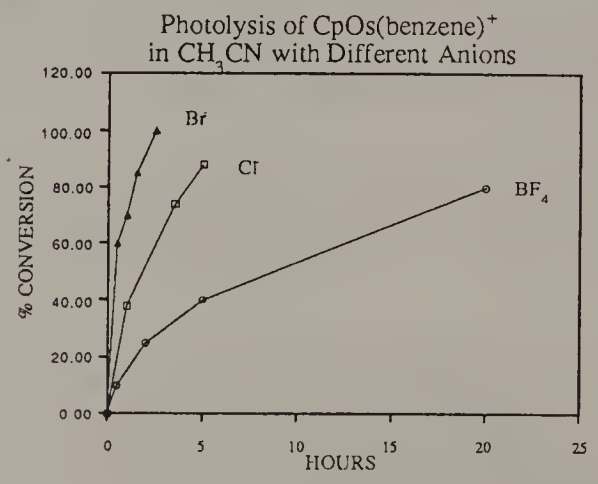
Photochemistry

The January issue of *Pure & Appl. Chem.* for 1995 has been devoted to publishing details of the 15th IUPAC Symposium on Photochemistry, held in Prague, Czech Republic, on 17–22 July 1994. This symposium was held under the chairmanship of Prof. J. Michl (University of Colorado, USA). The published papers reveal that a particularly wide range of topic, spanning physical photochemistry to biological photochemistry, were discussed in Prague.

At the conclusion of the symposium, the Porter Medal (named in honour of Lord (George) Porter) was awarded to the scientist deemed to have made the most significant contribution to photochemistry in the previous two years. This years recipient was Prof. N. J. Turro (Columbia University, New York, USA).

Probably the most important photochemical process on Earth is the light-harvesting process in green plants involving chlorophyll, i.e. photosynthesis, where sunlight is used to break water into its constituent atoms to reduce carbon dioxide. Prof. M. A. El-Sayed (Georgia Institute of Technology, USA) and co-workers presented a paper on the other important light-harvesting molecule – bacteriorhodopsin, On the Molecular Mechanism of the Rapid and Slow Solar-to-Electric Energy Storage Process by the Other Natural Photosynthetic System, Bacteriorhodopsin.

Upon absorption of solar energy by retinal in bacteriorhodopsin (bR), a rapid, and highly specific, photoisomerization of the retinal around the C(13)–C(14) bond takes place. This is followed by the formation of a number of intermediates, resulting from conformational changes of the protein around the retinal, which leads to the deprotonation of the protonated Schiff base of the retinylidene system. This is the switch of the proton pump which leads to the last step in the storage of solar energy in the form of electric energy by this photosynthetic system. The present authors find that removal of the metal cations from bR inhibits the process of deprotonation.



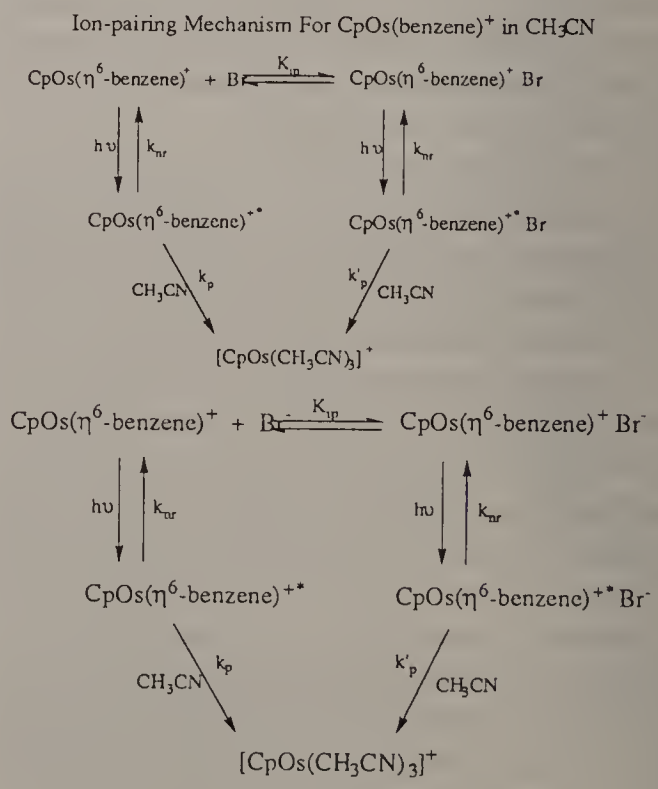


Figure 1 Photochemical reactions of CpOs(benzene)+ with details of derived mechanism'

Table 1. Principal photopolymer systems

Polymer concept	Main features	Applications
Classical:		
Acrylate/radical photoinitiator	Light penetration, photospeed	Resists, stereolithography
Epoxide/cationic photoinitiator	Low reaction shrinkage	Solder masks, stereolithography
Novolak/Diazoquin-one	Photosolublization	Photoresists for microelectronics
Combination systems:		
Acrylated polymide precursors	Photocrosslinking followed by thermal cure	Permanent layers in microelectronics
Epoxide/Acrylate hybrids	Combination of photospeed and low shrinkage	Stereolithography
New photopolymers:		
Auto-photosensitive polyimides	Direct photocrosslinking of a soluble fully imidized system	Permanent layers in microelectronics
Dimethylmaleic imide containing photopolymers	[2+2] photocycloaddition as photocrosslinking reaction	Textile printing, cartographic use
Photo-terpolymers	Chemically amplified photosolublization	Positive deep-UV microresists

In this paper, the authors summarize the results of their recent studies, together with those of other workers, regarding two important questions concerning the conversion process: (i) what is(are) the molecular mechanism(s) of the protein catalysis of the photoisomerization process and (ii) what is the role of the metal cations in the deprotonation process of the protonated Schiff base (the switch of the proton pump)? In order to answer the first question, the results of subpicosecond photoisomerization rate of retinal in bR and in a number of its relevant mutants were discussed in terms of steric and electronic factors. In an effort to answer the second question, the authors discuss the results of binding studies of Ca^{2+} to bR, to its mutants and to bR after it's C-terminus has been cleaved. From these results and the results, from the literature, on the ^{31}P NMR of Nd^{3+} regenerated bR, it is concluded that one or two metal cations strongly bound to the protein, but not on the surface, are functionally important. A model in which these metal cations control the pK values of the aspartic acids in the 85 and 212 positions and that of the protonated Schiff base during the photocycle is discussed.

A group from the Department of Chemistry, University of Minnesota, Prof. K.R. Mann *et al.* (Minneapolis, USA) have been investigating the mechanism for photochemical reactions involving the substitutionally inert, low spin d^6 $[CpM(arene)]^+$ complexes with simple arene ligands. The photochemical displacement of η^6-arenes from $CpM(\eta^6\text{-arenes})^+$ complexes, with M = Fe, Ru, Os, involves excitation to produce reactive, d-d excited states. The reactivity of these complexes is seen to decrease in the series Fe > Ru > Os for simple methyl substituted arenes. The quantum yields for these photoreactions indicate a significant associative component in the mechanism of arene release. The quantum yield for the Fe complexes can be varied by 10^6 by changing the steric hindrance, the solvent nucleophilicity and the nature of the counter ion. The synthesis, photochemical and photophysical properties of $CpM(\eta^6\text{-arenes})^+$ complexes (arene = rubrene, 9-phenylanthracene, coumarin laser dyes) have been investigated. In several cases (arene = rubrene, 9-phenylanthracene) emissive and non-emissive isomers were produced. $CpM(\eta^6\text{-arenes})^+$ complexes that exhibit fluid solution emission have metal complexation of a pendant rather than a chromophore arene ring. Photochemical arene decomplexation and emission quantum yields for the $CpRu^+$ complexes of substituted coumarins, rubene, and 9-phenylanthracene show that the reaction and emission quantum yields are inversely related. It is found that when the photo-active d–d states are below the emissive arene chromophore in energy, arene displacement is observed and when the arene localized chromophore energy is lowest, emission from the complex is observed.

From industrial laboratories working in photochemistry, there was a contribution by Dr N. Bühler and Dr D. Bellus of Ciba-Geigy, Basel, Switzerland, on polymer photochemistry. These authors showed that light far from being the ultimate source of energy for the various natural processes in biology, it is also the basis of much interesting modern technology.

Indeed, the use of light to produce polymers has a long history. As early as 1913, Klatte converted 50 tons of vinylchloroacetate into polyvinylchloroacetate by irradiation with sunlight in large glass vessels.

For industrial photochemists, the interaction of molecules with light not only offers a basis for many desired effects such as dyeing, pigmentation and optical brightening, but light also enables imaging within a wide span of new applications (microelectronics, printing wiring boards, information storage, display technologies, textile and printing processes). Indeed, one of the most exciting new developments is the design of new materials for microlithographic applications. Table 1 displays some of the current developments in industrial polymer photochemistry.

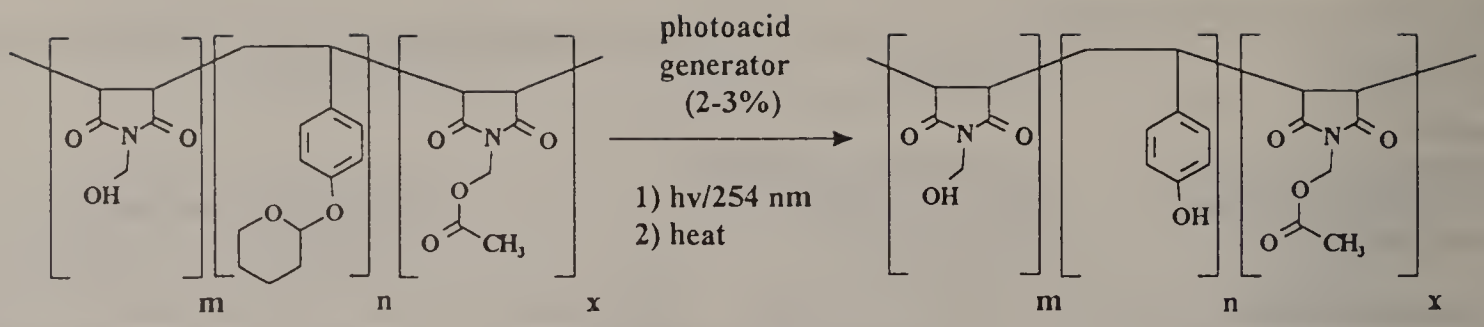


Figure 2. Photosensitive terpolymer approach and its photochemical deprotection.

Modern technology's continuing demands for new photopolymers necessitates the development of almost tailor-made materials with well-defined linear or non-linear optical response to incident light, higher resolution in optical lithography and inherent end properties of the cured material such as thermal stability, low reaction shrinkage and well defined mechanical and electrical properties.

How does one design such a material? Bühler and Bellus show us how some of these characteristics may be incorporated into new materials. The systematic study of the reaction of maleic anhydride with 2-aminopyridine in acetic acid rendered a one pot preparation of molecule 18 (Fig. 3) possible. This material was found to have two specific properties; firstly, an ability to undergo [2 + 2] cycloaddition under UV irradiation, and secondly, the reluctance of it's sterically hindered double bond to participate in radical or cationic polymerizations. This latter property allows an easy homo- or co-polymerization of acrylic monomers (19) to yield linear soluble polymers (20) with pendant dimethylmaleimidyl-groups. UV exposure of 20 in the presence of a photosensitizer such as thioxanthones yield cross-linked, insoluble polymers of type 21 (Fig. 3).

A wide variety of tailor-made polymers can be made with this approach. For example, a co-monomer methacrylic acid provides groups for subsequent dyeing by basic dyes as well as for the development of thin layers by a low-alkaline water-based process. Applied on a supporting film or aluminium sheet, such photopolymer coats of 2–3 μm thickness exhibit excellent resolution, dimensional stability and, especially noteworthy, no oxygen inhibition effects on photocrosslinking – they find much use in photolithographic applications.

Prof. Nicholas Turro (Columbia University, USA) gave a talk on the photochemistry of supramolecular systems. Supramolecular chemistry is concerned with molecular assemblages where stable covalently bound molecules assemble spontaneously into a larger scale structure through weak non-bonded interactions such as hydrogen-bonds or van der Waals forces.

Consider the 'cage effect' in liquids, and it's extension to the 'supercage effect' in micelles as an example of the development of supramolecular concepts and their application to produce novel and extensive supramolecular photochemical investigations. The 'guests' in the conventional cage effect are geminate radical pairs produced by a photochemical event, for example, the photochemically induced α-cleavage of triplet state ketones. This radical pair is 'localized' within the liquid because of the proximity of the solvent molecules. Consequently, their recombination is strongly dependent

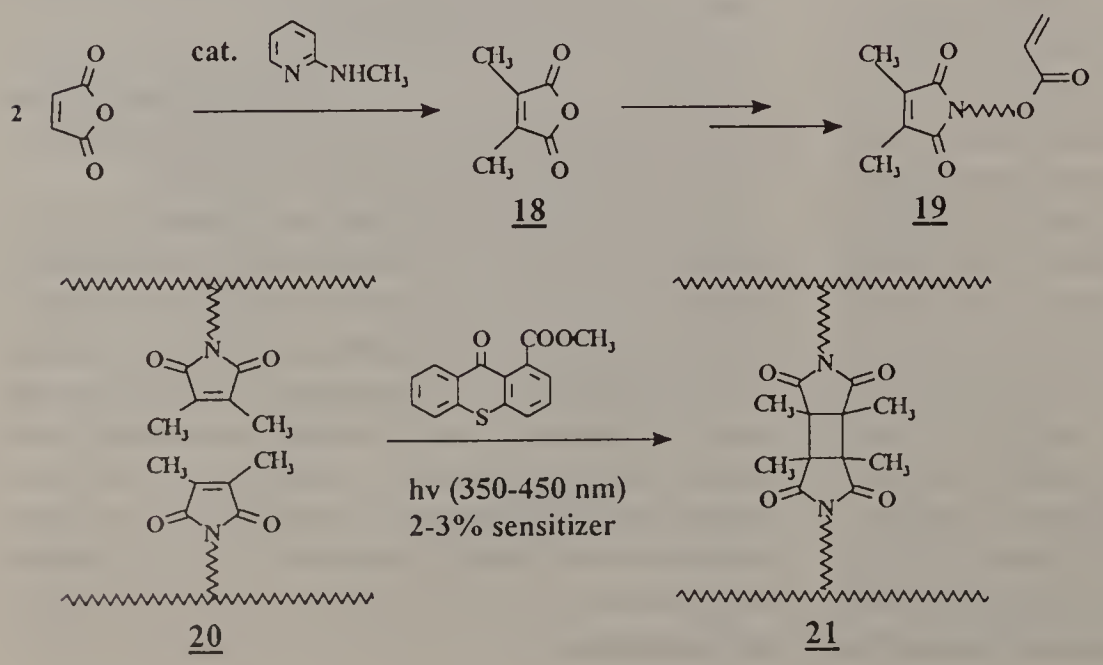
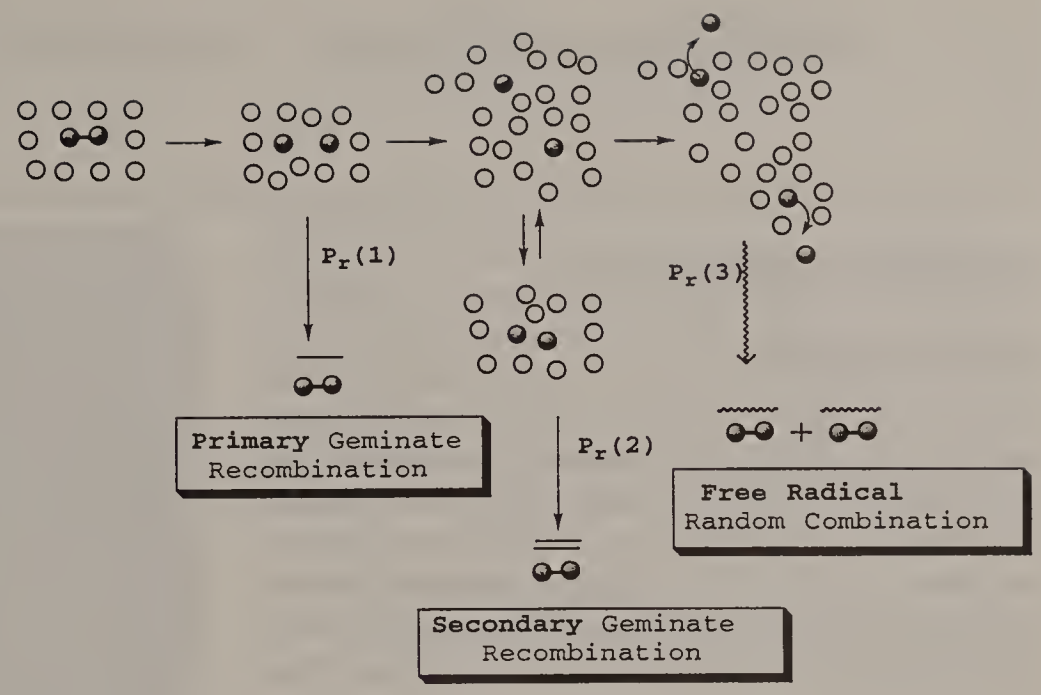


Figure 3. Synthesis of dimethylmaleic anhydride and its photochemical utilization.

Figure 4. Schematic description of the cage effect.



on the size of the cage within which they 'rattle' around. The 'host' in the molecular cage effect is thus the restricted space between solvent molecules and the 'host' in the 'supramolecular' cage effect is the restricted volume produced by, for example, a micellar aggregate.

The authors have investigated the recombination of radical pairs in micelle systems, they have set up various models and then experimentally characterized the parameters which enter their theoretical models (Fig. 4).

The other project reported by Turro *et al.* employed photoinduced electron transfer to investigate the structure and dynamics of supramolecular systems composed of metal complexes (guests) and anionic interfaces (hosts). The structures of the metal complexes which served as the donor and acceptor are derivatives of the familiar $M(bpy)_3^{n+}$ structure, with M = Ru, $n = 2$ as a donor and M = Rh, $n = 3$ as an acceptor.

The photoinduced transfer between donor and acceptor pairs of such metal complexes bound to three different anionic interfaces, micelles, starburst dendrimers, were investigated. From these studies, the authors have determined the mode of binding of the guest-host complexes and the rate constants for electron transfer as a function of binding mode, for example, hydrophobic or electrostatic, and the size and dimensionality of the host. For example, it was found that the rate of transfer between donor and acceptor as measured by nanosecond flash spectroscopy is very fast (10^9 s^{-1}) in a 15-base-pair piece of DNA (Fig. 5). This work suggests that the DNA molecule might be able to act as a molecular 'wire' (see p. 85).

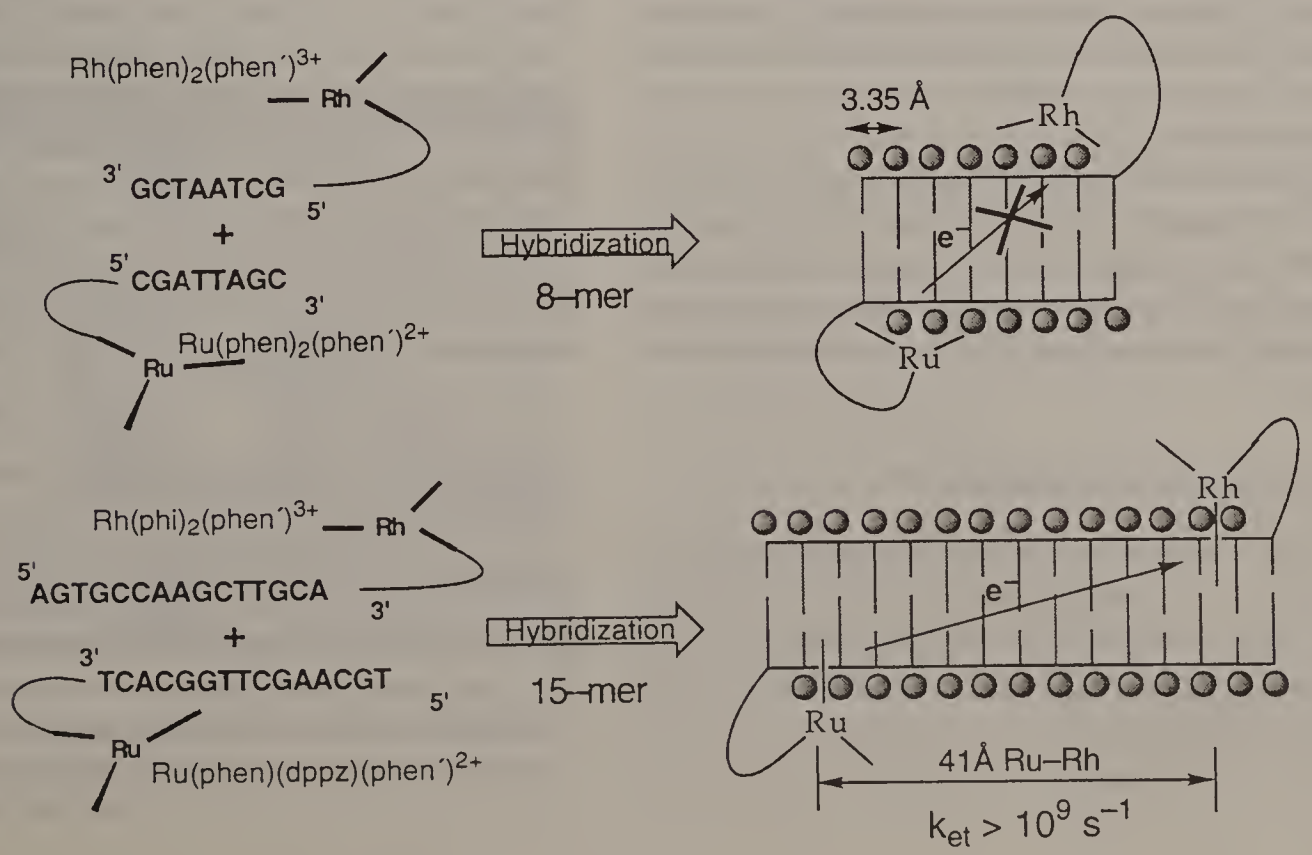


Figure 5.

Affiliate Affairs

Information for affiliates

IUPAC publications

Affiliates are entitled to a 25% reduction and in some cases a 40% reduction on the cost of IUPAC publications except the scientific journal *Pure and Applied Chemistry*. A leaflet detailing IUPAC books currently available from Blackwell Scientific Publications has recently been distributed by the publishers to all *CI* readers. Further copies may be obtained from the IUPAC Secretariat.

Ties and scarves

IUPAC ties and scarves may be purchased from the IUPAC Secretariat by applying to the Affiliate Affairs Secretary. The colours for both are *either* maroon *or* navy (dark) blue. The ties cost USD 14.00/GBP 7.00 each and the scarves USD 12.00/GBP 6.00 (including postage and packing).

Please use the form (or a photocopy of it) published on page 24 of the January 1994 issue of *CI*. Alternatively please write to the Affiliate Affairs Secretary with your order stating the colour you require. A cheque made payable to IUPAC for the appropriate amount should be enclosed with your order.

IUPAC poster

Copies of an IUPAC poster are available **free of charge** to affiliates and members of IUPAC's commissions and committees. The poster is printed in maroon and black on a white background and is approximately 42 × 59 cm in size.

IUPAC welcomes any publicity you can give to its activities. If you would like to display one or more copies of the poster in your department or elsewhere please write to the Affiliate Affairs Secretary stating your name and address and how many copies of the poster you wish to receive.

How to contact commissions

IUPAC affiliates are encouraged to communicate directly on scientific matters with the officers of IUPAC commissions. A full list of names and addresses of all commission officers for 1994–95 was published in the November 1993 issue of *CI*.

Address of IUPAC Secretariat

Please use the following address for all communications directed to the IUPAC Affiliate Affairs Secretary. If your are submitting a letter for publication in *Chemistry International* (*CI*), please indicate that the letter is 'Submitted for publication in *CI*.'

Affiliate Affairs Secretary, IUPAC Secretariat,
Bank Court Chambers, 2–3 Pound Way,
Templars Square
Cowley, Oxford OX4 3YF, UK.

Tel: +44 (1865) 747744;
Fax: +44 (1865) 747510
E-mail: iupac@vax.oxford.ac.uk

Affiliate reduction of conference registration fees

It is a condition of IUPAC sponsorship of a conference that IUPAC affiliates are entitled to a 10% reduction or 'own members' rate on the registration fee for scientific participants. This concession is usually, but not always, announced in the conference circulars and indicated on the registration form.

To receive this reduction an affiliate must declare on the conference registration form that (s)he is an affiliate. Alternatively the affiliate should apply in writing to the conference organizer for this reduction stating that (s)he is an affiliate. Conference organizers may check with the IUPAC Secretariat that applicants for this reduction are currently registered as affiliates.

If an application for this reduction is refused, an affiliate should immediately notify the Affiliate Affairs Secretary and, if possible, forward copies of documentary evidence of this refusal.

IUPAC-sponsored conferences

If you are interested in attending a conference please apply directly to the conference organizers for the conference circulars and registration forms. An updated list of names and addresses of the organizers of all future IUPAC sponsored conferences is given in the 'Conference Calendar' published in each issue of *CI*.

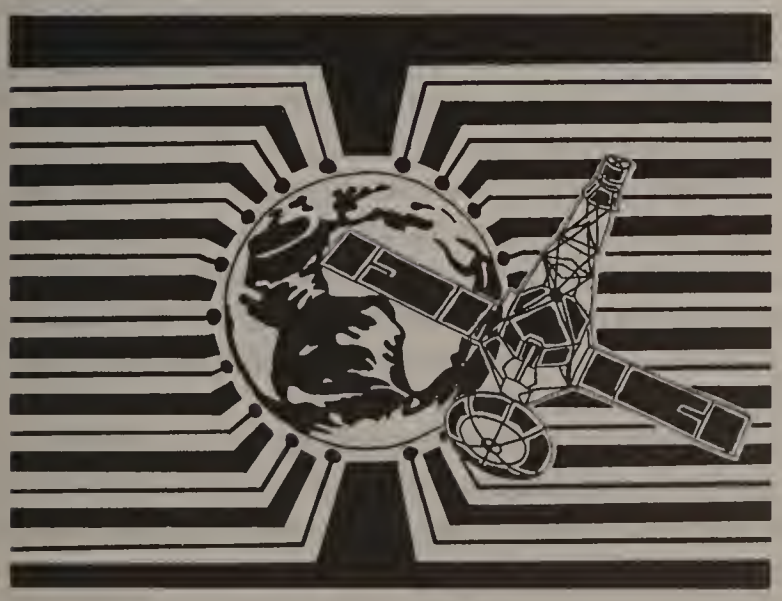
News and Views

A Glimpse of the Future

We are all familiar with large international conferences. Apart from the scientific program, they are an opportunity to renew old friendships and acquaintances, a chance to catch up on gossip as well as the latest news concerning the particular field of endeavour. Likewise, they are an occasion for the experts to meet, perhaps unofficially, and take policy decisions in a particular field and for younger scientists to make contacts and look for jobs. In all the many years of my own conference going, I have never been to an ugly or unpleasant location, the conference itself might have been exceedingly dull, but the location was always acceptable. One might therefore surmise that conferences also serve the purpose of giving semi-official, paid holidays to the participants.

However, all this might, however, be about to change. In November of 1994, 300 chemists from around the world attended a conference on computational chemistry. However, they were not gathered together in the large ball-room of an Alpine Skiing Hotel, or a conference center overlooking the Mediterranean. Rather they sat in their own offices viewing a computer screen and tapped out messages at a keyboard. Likewise, a group of 250 experts in chemometrics from around the world convened electronically from the end of September 1994 to early November 1994.

Both groups were participating in a revolution in the traditional manner for exchanging scientific information. These two electronic conferences were: the First Electronic Computational Chemistry Conference (ECCC) and the First International Chemometrics Internet Conference (InCINC'94). Gone are the days when scientists stood in front of an audience of other scientists and attempted, with varying degrees of success, to communicate with their audience. We are now entering the hypermedia universe (*C&E News* 12 December 1994).



The 'web' is a state-of-the-art communications medium that promises to greatly increase the scientists means of exchanging information.

These two ground-breaking conferences are important because, in comparison with earlier attempts at using computer conferencing, these two 'meetings' engaged the full potential offered by the Internet. In particular, they made use of the World Wide Web (WWW), commonly known as 'the web', the network-based document delivery system that links computers worldwide into a hypermedia universe.

The 'web' is a state-of-the-art communications medium that promises to greatly increase the scientists means of exchanging information. A client-server system on the Internet, the 'web', makes it possible for many computers to share the same single copy of a file stored in the server, rather than having copies distributed among numerous computers in different locations. A 'browser' is used to manoeuvre the user through the 'web'. For most personal computer systems, Macintosh and Windows, the most widely used 'browser' is 'Mosaic' (developed at the National Center for Supercomputing Applications, University of Illinois, US). 'Mosaic' may be down loaded from the Internet free of charge.

To pilot a user around the Internet, the 'web' employs a technique called hypertext. Here, a word, a phrase or an icon in a particular document is highlighted. By using the mouse to identify this label, a user activates coding messages embedded in the document that direct the 'browser' to move to some other point in the document or to call up another document, either locally, for example, from the same or another paper at the same conference, or somewhere else in the world. The system is essentially a very sophisticated key-word, key-phrase or even key-figure search package, but accessing all available on-line literature.

ECCC and InCINC'94 were not the first 'on-line' conferences. That honor belongs to a computer conference on Applications of Technology in Teaching Chemistry (14 June – 20 August 1993), sponsored by the American Chemical Society. This meeting had only 15 'papers', however, it drew 450 registrants from 33 countries. These 'papers', on applications of computers, networks and telecommunications in chemical

education were transmitted primarily by E-mail In addition, graphics, text, software and discussion transcripts could be accessed by direct file transfer from the main computer system where they were stored. Use of the 'web', due to the availability of a client-server system for multiple user interactive access, adds a new dimension to the electronic conferencing format.

Prior to the commencement of the ECCC meeting, all the 'papers' were made available on the 'web'. Not only could the text be viewed, but also the full-colour graphics, diagrams and molecular models, along with video for motion and even audio were available. This computational chemistry conference was organized to explore the potential use of the Internet by the international chemistry community. It was sponsored by the Camille & Henry Dreyfus Foundation and had a scientific organizing committee to ensure that only the best science was presented.

InCINC'94 ran for 8 weeks and was sponsored by the International Chemometrics Society and the international publishing house Elsevier, who are particularly active in on-line electronic publishing. Conference organizer Barry M. Wise (Pacific Northern Laboratory) divided the program into weekly thematic sessions, each treating an average of three to five papers. participants viewed the 'manuscripts' and then sent comments and questions by E-mail to the authors and each other. According to participants (*C & E News* 12 December 1994), the conference was, 'a head-spinning mix of intermingled, simultaneous conversations – ranging from mundane questions about accessing files to elegant theoretical discourses'. Many conference participants found themselves spending a great deal of time 'plugged in', digesting 'papers', reading comments and composing remarks. Presenters had two options for submitting their presentations. They could place them along with the supporting graphics and other files on their own servers for connection through the main server of the conference. Or they could transmit all documents to the main conference server for placement there.

One of the ideas behind the conference was that ECCC resemble an on-line poster session. However, some of the advantages of the poster session, such as personal or one-to-one interactions cannot be translated directly. But, as with traditional poster sessions, attendees should be able to leisurely view the posters in which they are interested and discuss aspects of the posters' contents with the presenters. Presenters need a flexible, unrestricted means for preparing their posters that might contain text, graphics, audio and video, in addition to having the ability to discuss their work with other presenters.

The organizing committee expects the CD-ROM of the ECCC proceedings to expand on one of the conference's goals. That of exploring new avenues for the dissemination of technical information. Versions of the CD-ROM for Macintosh and Windows computers will contain all the 'papers' and the E-mail discussions. They will also contain the 'web' 'browsers' and viewers to make them 'plug-and-play' products. In addition, Chemical Abstract Service has tentatively agreed to abstract the presentations.

The on-line conference has many advantages over the more traditional 'stand-up and talk' conference. In a conventional meeting, you have a small number of exchanges of easily forgotten comments. The on-line meeting provides a complete record of all comments, not subject to space or time requirements. Unfortunately, these comments have neither been filtered nor edited. Traditional conference proceedings might be considered by many as slow and old-fashioned, however, they have been peer-reviewed and edited.

For the majority of participants, however, the great advantage, apart from the flashy new computer technology, is the possibility of participating in a major conference and staying at home. Indeed, one is able to participate in the conference at one's own speed. One can read, formulate questions and make comments at your own pace rather than at the pace of the speaker, or the timetabling of the chairman, as in a traditional conference. Such electronic conferences open up the field to people who could not, or would not, normally attend – especially with travel cutbacks currently facing many research organizations. With communication over the Internet, the expertise and opinions of researchers around the world becomes available without the necessity of paying their travel expenses to some idyllic, but out-of-the-way location. Experts need not take time off from their work and relocate themselves. This facility will undoubtedly benefit those conferences which seek to unit scientists from Australia and Europe with their American and Japanese colleagues. However, as noted by some of the participants at ECCC, the intercontinental telephone line is slow and got even slower when the conference began. A global conference would either have to have faster phone lines or a host computer on each side of an ocean.

At the moment, this technology is emergent and there will undoubtedly be many teething problems to overcome in setting up truly global conferences. However, from the point of view of the International Union of Pure and Applied Chemistry, this type of electronic conference could benefit us enormously. The Union is an organization which, to fulfil its remit, requires small groups of experts, from many countries, to come together and formulate ideas and come to decisions on matters of nomenclature, classification and policy. To pay for this important work, the Union has only limited funds, and this limits the number of meetings of the various IUPAC committees and therefore limits the speed with which final decisions are arrived at. Perhaps for the

Union, as a means of stretching its travel budgets, the future lies in electronic conferencing. One would of course need to ensure that suitable computers were available, however, the gains to be made in savings on travel and subsistence might well be enormous.

Also, the advent of electronic conferencing would greatly assist the publication and dissemination of final documents. If the final version of a document exists as a file in a computer, it is trivial to send it to another computer for publishing and storage. I suspect that we would all benefit from such an abolition of paper.

The arriving dominance of the computer as a means of rapid international communication can also be seen in recent developments at Oxford University Press.

Alarmed that scientists are exchanging research findings on computer-linked electronic bulletin boards, rather than seeking to publish their results using the time-honoured peer-review method, Oxford University Press (OUP) is to begin distributing its journals on Internet, the global information network. The experiment is part of a wider bid by certain academic publishers to claim Internet as a formal paid-for publishing medium. At present, users pay for the communications link to Internet, but the information is free.

Internet represents a new way of rapidly exchanging vast amounts of data, apparently, there are many thousands of gigabytes of information transmitted over the system daily, without the intervention of publishing companies. OUP, which has been publishing since 1478, feel that professional publishing organizations need to get involved in the Internet to bring some order to the un-edited chaos of the present global exchange of information.

Publishing on Internet will allow OUP to customize the previously stable paper information into a more dynamic product, with each user being able to order what it is they actually wish to purchase. To reach this flexibility, OUP is first moving to the publication of its 140 journals on CD-ROM as well as on paper.

OUP is apparently convinced that electronic publishing is the way of the future and that with the need to be first 'in print' with important new results, the best scientists will increasingly chose to publish on the Internet. With its twice monthly *Nucleic Acid Research*, for example, OUP will, by publishing on the Internet, cut three weeks from the current 12-week cycle from acceptance of a paper to publication.

OUP's move marks a wider recognition among publishers that their product is information, not books and journals, and that electronic publishing technology gives them the power to manipulate that body of information. Academic journals have a relatively stable market, so rather than expand the subscriber base, the added value is intended to keep existing subscribers loyal. Subscription prices will not be markedly different, but the CD-ROM journal will be easier to use than the old paper version. It is estimated that only 5% of the information in any one journal is directly relevant to an individual scientist. And that many readers do not have the time to find that important 5%. With the journal online, it will take only seconds to find what any particular wants. Likewise, literature searches become trivial and not intimidating.

Via Internet, one could send abstracts and headline information about upcoming publications. Users could then order only what is of interest to them, rather than take the whole paper journal.

Again, considering the huge amounts of information, in a variety of fields, published each year by IUPAC, such Internet publications are perhaps something that we should be considering.

Changes at the Oxford Secretariat

At the end of March, Miss Ann Troughton retired from her IUPAC post as Deputy Executive Secretary, having joined the Secretariat staff as Assistant Secretary in 1975. During these twenty years she was responsible for successfully organizing the ever larger and more complex biennial General Assemblies of the Union – a not inconsiderable problem of logistics, and long-range and long-distance planning. Also, Ann was the central contact person for the various Divisions/Sections, Commissions, and other IUPAC bodies, in respect of their memberships, finance, meetings, and projects. She oversaw a change from the traditional *Comptes Rendus* from each Assembly to the present *IUPAC Handbook*. Ann will continue on a part-time basis until the end of this summer, 1995, in order to ensure continuity for the 38th Assembly (Guildford, UK: 4–11 August 1995) and to help with the initial planning for the Assemblies in 1997 and 1999.

A restructuring of the Secretariat staff is at an advanced stage, and details will be announced shortly.

Ann Troughton

Prof. Paul Knochel receiving a medallion from Prof. C.N.R. Rao (a past President of IUPAC) after having received the Thieme-IUPAC Prize for Organic Synthesis.

Thieme–IUPAC Prize in Synthetic Organic Chemistry 1994

The details of the recipient, Prof. Paul Knochel, and of the work, for which he was awarded the 1994 Thieme-IUPAC Prize for Synthetic Organic Chemistry have been published in *Chem. Intl.* 230 16 (1994). Prof. Knochel received his prize in Bangalore, India, at the Tenth International Conference on Organic Synthesis, December 1994.

Element 111

A collaboration between the *Gesellschaft für Schwerionenforschung (GSI)* in Darmstadt, Germany, the Flerov Laboratory of Nuclear Reactions at Dubna, Russia, the Department of Nuclear Physics, Comenius University in Bratislava, Slovakia, and the Department of Physics of the University of Jyvaskyla in Finland have recently announced experimental evidence for the creation of element 111.

In the last issue of *Chemistry International* we reported on the discovery by nuclear scientists at the GSI, Heavy Ion Research Center, Darmstadt, Germany, of element 110. Now, almost a month to the day after they had announced their discovery of element 110, the same group has announced the discovery of element 111. The international team, lead by Prof. Peter Armbruster, has succeeded in creating three atoms of element 111 by fusing nuclei of nickel and bismuth.

In an experiment to identify element 111, the scientists observed an alpha-decay chain that can be unambiguously assigned to the specific isotope of element 111. These experiments involve accelerating one of the atoms, ^{64}Ni, which has been stripped of its electrons, and colliding this accelerated particle into an appropriate target, here ^{209}Bi. It was found that these data result in the generation of element 111 in the reaction ^{64}Ni + ^{209}Bi $\rightarrow$ ^{272}111 + neutron.

The idea is to produce the new nucleus with as little excitation as possible – cold fusion. This occurs when the projectile ion is given just enough energy, electrostatic acceleration of the ion in an applied laboratory field, to overcome the electrostatic repulsion of the target nucleus, producing a super-heavy nucleus with little residual energy.

Further observations showed a subsequent decay chain of 4 consecutive alpha-decays. Thus, it is reasonable that the originally formed nucleus could be assigned to the isotope of mass 272 of element 111 (on the basis of alpha-decay coincidences). The isotope ^{272}111 is seen to decay with a half-life of 1.5 milliseconds by emission of α-particles (^{4}He).

The new element is not created very rapidly. According to Armbruster, an average of 10^{18} accelerated nuclei strike the cooled targets before one successful event occurs. Most of the accelerated ions pass straight through the target.

The decay chain may be written:

^{64}Ni + ^{209}Bi $\rightarrow$ ^{272}111 (unstable compound nucleus)
$\rightarrow$ ^{268}109(meitnerium) + α-particle
$\rightarrow$ ^{264}107(bohrium)+ α-particle
$\rightarrow$ ^{260}105(joliotium) + α-particle
$\rightarrow$ ^{256}103(lawrencium) + α-particle

The GSI experiment not only led to the creation of element 111 but also to the creation of new isotopes of elements 107 and 109 with masses 264 and 268, respectively. Armbruster adds that in creating elements 110 and 111, 'we also found a second isotope for element 110 with mass 271.' These experiments provide nuclear scientists with invaluable information about the stability of elements with high atomic numbers and variable nuclear structure (differing neutron number) – theoreticians have long predicted that above a certain atomic number there will be a filled nuclear shell and such elements will be much more stable than their very heavy element predecessors in the Periodic Table – an island of stability.

Measuring Solute Diffusion Coefficients Rapidly

Researchers in Russia and Italy have developed a straightforward method for rapidly measuring the diffusion coefficients for both large and small molecules in solution. The method has the advantage that it uses apparatus routinely found in biochemical laboratories.

Many years ago, Geoffrey I. Taylor proposed an explanation for his observation of the dispersion, or diffusion, of a solute in the direction perpendicular to the direction of flow of a solution, containing that solute, flowing through a pipe of uniform cross-section.

The velocity of a fluid flowing slowly through a tube (laminar flow) varies over the tube cross-section. For a cylindrical tube with a circular cross-section, the veloc-

ity is a parabolic function of the radius, reaching a maximum on the tube axis and approaching zero at the tube walls. Solute particles or molecules introduced into the flowing fluid move with the fluid at different velocities corresponding to their positions at the tube cross-section. Moreover, molecular diffusion redistributes them over both the tube cross-section and the tube axis. Interaction of the non-uniformity of the fluid velocity and the molecular diffusion leads to a specific mechanism of dispersion termed Taylor dispersion.

The problem was analyzed for non-uniform pipe cross-sections by Aris, and such diffusion or dispersion processes are now termed Taylor–Aris dispersion. The approximations adopted led to the conclusion that the mass flux along the tube axis (Q) may be represented as a sum of a convective part and a diffusion part given by Fick's law with an apparent diffusion constant D*

$$Q = UC_m + D^*(\partial C_m/\partial x),$$

where U is the mean velocity, C_m is the analyte concentration over the tube cross-section and x is the distance along the tube axis.

The apparent diffusion constant, D* is related to the tube radius (R), the mean velocity of the fluid and the coefficient of molecular diffusion (D). The full theory of Taylor–Aris dispersion leads to the simple expression for D*:

$$D^* = D + (R^2U^2/48D).$$

This simple equation provides a basis for obtaining the molecular diffusion constant for a solute molecule through an experimental measurement of its dispersion coefficient D* in a fluid flow of known mean velocity flowing through a tube of known diameter.

The new method of determining dispersion coefficients, which relies upon Taylor–Aris dispersion, was developed by Michael Bello at the Institute of Macromolecular Compounds, St Petersburg, and Roberta Rezzonico and Pietro Righetti at the University of Milan, Italy. It uses a commercially available capillary electrophoresis instrument equipped with a pump, injection system and a detector capable of monitoring the presence and concentration of the solute under investigation (normally a UV source and detector to monitor solute absorption) connected to a computer for analysis (*Science* **266**, 773 (1994)).

In the electrophoresis tube, a constant applied voltage causes the electrolyte solution to flow in a constant laminar manner through the tube. Thereby setting up the velocity gradient which in Taylor–Aris dispersion will cause the solute molecules to diffuse. Thus, at the entrance of the tube one adds a narrow band of solute molecules, these disperse as they flow through the tube in the electrolyte. The observed dispersion, under the known laboratory conditions, yields the diffusion coefficient.

The authors have tested their method with a wide distribution of solutes; potassium hydroxide solution, citric acid, phenylalanine, tryptophan, haemoglobin and ovalbumin in aqueous or buffer solutions. Where the values for the diffusion coefficients are available in the literature, the agreement is seen to be very good. The experiments are quick and have the potential for giving detailed information as a function of solution pH, temperature and solute concentration.

The diffusion coefficient of a macromolecule is an important quantity in biochemical and biophysical measurements because this property is usually related to the molecular shape and to its mass. The present method of determining coefficients of diffusion is based on readily available laboratory equipment and allows an easy, rapid and reproducible determination of D values for both large macromolecules and small analytes. An additional advantage of the present method is that only small volumes of solution, fractions of nanolitres, are required.

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* **15**, 215–227 (1993). The IUPAC Secretariat have been notified of the following changes:

Prof. Allen J. Bard, E-mail: ajbard@mail.utexas.edu

Prof. G. den Boef, E-mail: gdboef@anal.chem.uva.nl

Prof. W.-D. Busse, Fax: (49) 202 364471

Prof. Anne-Marie Cazabat, E-mail: cazabat@ext.jussieu.fr

Prof. James Economy, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, 1304 W. Green Street, Urbana, IL 61801, USA, E-mail: festes@uxl.cso.uiuc.edu.

Dr J.L. Fox, 3100 Woodgreek Drive, Downers Grove, IL 60515, USA. E-mail: larryfox@nap.amoco.com

Dr John Herron, E-mail: herron@enh.nist.gov

Prof. Willem H. Koppenol, E-mail: koppenol@inorg.chem.ethz.ch

Dr R. P. Martin, Fax: (33) 1 49 55 13 18

Dr John R. Moody, NIST, Building 222, Room B-212, Gaithersburg, MD 20899, USA. Tel.: (1) 301 975 4134, Fax: (1) 301 977 0587, E-mail: jmoody@micf.nist.gov

Dr David S. Moore, E-mail: moored@lanl.gov

Prof. J.-C. Richer, E-mail: richerjc@ere.umontreal.ca

Prof. Pieter Steyn, Tel.: (27) 148 299 2340, Fax: (27) 148 299 2344, E-mail: chepss@puknet.puk.ac.za

Prof. Klara Tóth, Tel.: (36) 1 204 1111 ext. 2273

Dr William Work, E-mail: rbpwjw@rohmhaas.com

Publications

United Nations Environment Program(UNEP)

The Industry and Environment Program Activity Center (IE/PAC) was established in 1975 to bring together industry and government to promote environmentally sound industrial development.

UNEP has released, March 1994, a new Training Manual: Landfill of Hazardous Industrial Wastes (Technical Report No. 17).

Both newcomers and professionals working in the field of hazardous waste management will find this new UNEP IE/AC publication of great interest. It simulates and then analyzes landfill problems and options faced by many governments. The case study, reference information and problem solving exercises which may be found in this document can be used as the basis for realistic training courses and teaching programs. A model training workshop is described in the appendices. Technical information on industrial landfills, on hazardous waste management in general, as well as a useful resource package on how to carry out a waste survey are included.

The manual is structured around a case study which simulates an actual hazardous waste landfill. Problem-solving sessions which are described in the text include:

- Identification of waste for landfills;
- Siting of landfills;
- Engineering aspects;
- Operation and management;
- Regulatory procedures;
- Landfill closure and rehabitation.

Sufficient reference material is included to allow the exercises to be completed either in a group session or by individuals.

The manual was produced in collaboration with the International Solid Waste Public Cleansing Association (ISWA) and may be obtained (USD65.00 or FRF350.00, ISBN 92 807 13841, UN Sales No. 93-III-D3) from: UNEP IE/PAC, Tour Mirabeau, 39–43 quai André Citroën, 75739 Paris Cedex 15, France.

Molten Salts Bulletin *´Sels Fondus´*

The latest bulletin, 1994 No.55, in this series has been produced and contains a recent bibliography and details of recent conferences devoted to the study of molten salts. To continue this series of publications, interested readers are requested to send information and reprints concerning their work in this field to:

Molten Salts Bulletin Sels Fondus, M. Gaune-Escard, Institut Universitaire des Systèmes Thermiques Industriels, UA 1168, Université de Provence, Centre St. Jérôme, 13397 Marseille Cedex 20, France.

Pesticide Chemistry: Options 2000

The scope of pesticide chemistry embraces a wide variety of disciplines and extends far beyond the bounds of pure chemistry. Responding to the challenge of providing new molecules to control pests, was initially a straightforward task with high rates of both scientific and commercial success. The history of outstanding achievements in controlling disease vectors and crop pests has continued for many years. Even with dramatic advances in new chemistry and methods of delivery, pest control practitioners must today confront the problem of providing suitable control techniques for pest species in which the appearance of resistance to chemical controls may rapidly negate many years of effort. In addition, public concerns about the safety of materials released in large quantities into the environment demand that chemical approaches do not adversely affect society.

IUPAC has sponsored congresses in pesticide chemistry, at four yearly intervals, for the last 32 years. The Eighth International Congress of Pesticide Chemistry, organized by the American Chemical Society, was held in Washington, DC, in July 1994. The theme was the options for pest control chemistry as we enter the new century. The Programme Committee selected 10 major topics and these areas became the basis for the congress symposia. These areas are:

- Synthesis;
- Delivery;
- Environmental fate and behaviour;
- Residues;
- Biotechnology;
- Metabolism;
- Mode of action;
- Resistance;
- Regulation;
- Risk assessment.

The Eighth International Congress of Pesticide Chemistry: Options 2000, ISBN 0-8412-2995-3, eds N. N. Ragsdale, P. C. Kearney and J. R. Plimmer, is published in the Conference Proceedings Series of the American Chemical Society, Washington, DC, 1995. Price USD109.95 and may be ordered through the ACS, Distribution Office, Dept 321, PO Box 57136, Washington, DC 20037, USA.

The World Health Organization

The World Health Organization Environmental Health Criteria Series was launched in 1976 in response to concern over the risks to human health and the environment posed by the growing number of chemicals on the market and present in the environment. In planning the series, the aim was to give national authorities all the information needed to understand the specific hazards posed by a particular chemical and how to devise appropriate protective measures, whether for the health of workers, the safety of the general public, or to minimize destruction of the environment.

The Environmental Health Criteria (EHC) monographs produced by the International Program on Chemical Safety include an assessment of the effects on the environment and on human health of exposure to a chemical or combination of chemicals, or physical or biological agents. They also provide guidelines for setting exposure limits.

The purpose of a Health and Safety Guide (HSG) is to facilitate the application of these guidelines in national chemical safety programs. The first three sections in a particular HSG highlight the relevant technical information in the corresponding EHC. Section 4 deals with advice on preventive and protective measures and emergency action; health workers should be thoroughly familiar with the type of information found in this section. The section on regulatory information has been extracted from the legal file of the International Register of Potentially Toxic Chemicals (IRPTC) and from other United Nations sources.

Five new guides have recently been published:

- Health and Safety Guide No. 86, Methyl bromide (ISBN 92 4151086 2);
- Health and Safety Guide No. 87, Chloroform (ISBN 92 4151087 0);
- Health and Safety Guide No. 88, Phenol (ISBN 92 4151088 9).
- Health and Safety Guide No. 89, Tri-Allate $C_{10}H_{16}Cl_3NOS$ (ISBN 92 4 151089 7).
- Health and Safety Guide No. 90, Acetaldehyde (ISBN 92 4 151090 0).

Published by the World Health Organization for the International Program on Chemical Safety. These publications are priced CHF5 in developed countries and CHF3.5 in developing countries. Further information and copies from: Distribution and Sales, World Health Organization, 1211 Geneva 27, Switzerland.

Multiphoton Processes, Series in Optics and Photonics, Vol. 6

This volume contains the papers presented at the Sixth International Conference on Multiphoton Processes, held in the Laval University, Quebec, Canada. This series of conferences continues to alternate between Europe and North America, with the Seventh in the series scheduled for Germany in 1996.

The investigations of the interactions of intense laser beams with atoms and molecules continues to evolve. In the early days, that is to say some 15 years ago, the focus would have been on interactions of molecules with beams of light which today would be considered relatively weak. There has been, and continues to be, significant development in laser technology. Indeed, the horizon for research in the area of high-field laser interactions has shifted following the dramatic increase in achievable field strengths, and thanks to advances in ultrafast intense laser technology. Thus, the traditional perturbative approach to multiphoton processes is replaced by non-perturbative theories. These change are reflected in the current set of papers. This collection of papers with their references should provide a good update of the field and the state of the art in the area.

High-order harmonic generation in gases has been an active field of research for many years, because it not only provides a probe for investigating the mechanism of interaction between the light field and the atom or molecule under irradiation, but also because of the possibility of developing new coherent vacuum ultraviolet sources.

A new technique of photoelectron imagery in intense laser fields was described. Here colourful images of electrons ejected in the focal volume of a strong laser pulse after multiphoton ionization were shown. This technique projects expanding clouds of electrons with different initial kinetic energy distributions onto a microchannel plate.

Another important new technique is that of laser control of molecules using multiphoton chemistry, ultrafast laser science and high-field physics. At ICOMP VI, K. R. Wilson gave a talk on the focusing of wavepackets in molecules through ultrashort laser pulse chirping, P. Brumer discussed the theory of laser coherent control, A. Giusti-Suzor talked about weak and strong laser field control of H_2^+ dissociation using a two-colour phased locked technique and T. T. Nguyen-Dang showed the result of calculations on time-resolved control (tracking) of population in a 2-channel molecular system.

Proceedings of the Sixth International Conference on Multiphoton Processes, Université Laval, Québec, Canada, 25–30 June 1993. Eds D. K. Evans and S. L. Chin, World Scientific 1994, ISBN 981-02-1586-X.

International Newsletter on Chemical Education (INCE)

In the December 1994 issue (No.42) of *International Newsletter on Chemical Education*, Luis Bello concentrates on how to develop practical chemical skills for

chemists in Cuba and L. S. Sierra *et al.* look at the use of computers in training chemistry teachers in Cuba. Derry Jones considers links between industry and education in science and technology as revealed at a NATO Science Advanced research Workshop entitled *Advanced educational technology in school-industry link projects*. R. Ouahes has some interesting comments on the Periodic Table of the elements, 'Is the Periodic Table really periodic?'

Y. Marcus discusses the ideas on a *Eurocurriculum on analytical chemistry* produced by the working party on analytical chemistry of the Federation of European Chemical Societies. Due to the importance of analytical chemistry in modern society, the Federation of European Chemical Societies have produced a list of subjects with which an analytical chemist should be familiar. This basic curriculum includes:

- General topics (aims, processing, sampling, evaluation, literature);
- Chemical Analysis;
- Physical Analysis (IR, Raman, NMR, Auger, etc.);
- Computer-based analysis (chemometrics, signal processing, pattern recognition, etc.),

Y. Wu looks at the use of chemistry textbooks in chemistry education in China, *Analysis and survey of the new chemistry textbook for the nine year program of compulsory education in China.*

Peter J. Towse, Editor *INCE*

CSSE, University of Leeds, Leeds LS2 9JT, UK

Advisory Committee on Chemicals of Environmental Importance

The Advisory Committee on Existing Chemicals of Importance to the Environment (*Beratergremium für Umweltrelevante Altstoffe – BUA*) was established by the German Chemical Society in May 1982 in collaboration with the German Federal Government, the German scientific community and German chemical industry. BUA now has some 13 years of experience in working and estimating the environmental impact of commonly used chemicals. It has already published reports, in both English and German, on more than 180 chemicals. Recently, because of the importance of European Union legislation on the control of chemicals in the environment, BUA has set up links with the European Union. Within the EU, the first priority list of 43 common chemicals has recently been adopted.

The results of the Fifth BUA Colloquium are now published in English and can be ordered from the BUA Secretariat, PO Box 900 440, D-60444 Frankfurt am Main, Germany; Tel.: (49) 697917 331, Fax: (49) 69 7917 322

Please refer to: Gesellschaft Deutscher Chemiker, Monograph No.3, Assessment of Existing Chemicals 1995.

Topics include:

- Introduction; Report of the activities of BUA, Existing Substance Regulation 793/93;
- Risk assessment in the EU in the context of Regulation 793/93;
- The role of ECETOC within European and International Chemical Programs;
- Use of quantitative structure-activity relationships in the evaluation of existing substances;
- Priority settings by BUA and EU; results and experience;
- Evaluation of substances groups for priority setting.

Also available: *Gesellschaft Deutscher Chemiker*-Monograph No. 1 *Bewertung des ökologischen Gefährdungspotentials von Chemikalien*, German, 117 Pages, 1994. Both of these monographs are available at DEM 30 each.

Brochure: Assessment of existing chemicals: A contribution towards improving the environment, English, 48 Pages, 1992 (free).

Standards Published

New International Standards published between 6 August 1994 and 14 September 1994.

**French version of standard previously published in English only.

TC 28	**Petroleum products and lubricants**
ISO 8754: 1992**	Petroleum products – Determination of sulfur content – Energy-dispersive X-ray fluorescence method
TC 34	**Agricultural food products**
ISO 3496:1994	Meat and meat products – Determination of hydroxproline content
ISO 7701: 1994	Dried apples – Specification and test methods
ISO 11052: 1994	Durham wheat flour and semolina – Determination of yellow pigment content
TC 35	**Paints and varnishes**
ISO 8130-8: 1994	Coating powders – Part 8: Assessment of the storage stability of thermosetting powders
ISO 11341: 1994	Paints and varnishes – Artificial weathering and exposure to artificial radiation – Exposure to filtered xenonarc radiation
TC 45	**Rubber and rubber products**
ISO 705:1994	Rubber latex – Determination of density between 5°C and 40°C
ISO 7663: 1994	Rubber, halogenated isobutene- isopretene (BIIR and CIIR) – Evaluation procedure
TC 61	**Plastics**
ISO 307: 1994	Plastics – Polyamides – Determination of viscosity number
ISO 2818: 1994	Plastics – Preparation of test specimens by matching
TC 79	**Light metals and their alloys**
ISO 10074: 1994	Specification for hard anodic oxidation coatings on aluminium and its alloys
TC 85	**Nuclear energy**
ISO 11483: 1994	Preparation of plutonium sources and determination of 238Pu/239Pu isotope ration by alpha spectrometry
ISO 12184: 1994	Determination of solubility in nitric acid of plutonium in unirradiated mixed oxide fuel pellets $(U,Pu)O_2$
TC 121	**Anaesthetic and respiratory equipment**
ISO 5360: 1993**	Anaesthetic vaporizers – Agent-specific filling

	systems
ISO 8835-2; 1993**	Inhalational anaesthesia systems – Part 2: Anaesthetic circle breathing systems
TC 131	**Fluid power systems**
ISO 4400: 1994	Fluid power systems and components – B. Three pin electrical plug connectors with earth contact – Characteristics and requirements
ISO 6020-3: 1994	Hydraulic fluid power – Mounting dimensions for single rod cylinders, 15 Mpa (160 bar) series – Part 3; Compact series with bores from 250 mm to 500 mm
ISO 6952: 1994	Fluid power systems and components – Two-pin electrical plug connectors with earth contact – Characteristics and requirements
TC 132	**Ferroalloys**
ISO 10386: 1994	Ferroboron – Specification and conditions of delivery
ISO 10387: 1994	Metal chrome – Specification and conditions of delivery
TC 147	**Water quality**
ISO 7827: 1994	Water quality – Evaluation in an aqueous medium of the 'ultimate' aerobic biodegradability of organic compounds – Method by analysis of dissolved organic carbon (DOC)
ISO 7887: 1994	Water quality – Examination and determination of colour
ISO 11083: 1994	Water quality – Determination of chromium(VI) – Spectrometric method using 1,5-diphenylcarbazide
TC 27	**Solid mineral fuels**
ISO 7404-1: 1994	Methods for the petrographic analysis of bituminous coal and anthracite – Part 1; Vocabulary
ISO 7404-3: 1994	Methods for the petrographic analysis of bituminous coal and anthracite – Part 3; Method of determining maceral group composition
ISO 7407-5: 1994	Methods for the petrographic analysis of bituminous coal and anthracite – Part 5; Method of determining microscopically the reflectance of vitrinite
TC 28	**Petroleum products and lubricants**
ISO 3104: 1994	Petroleum products – Transparent and opaque liquids – Determination of kinematic viscosity and calculation of dynamic viscosity
TC 30	**Measurement of fluid flow in closed conduits**
ISO 10790: 1994	Measurement of fluid flow in closed conduits – Coriolis mass flowmeters
TC 34	**Agricultural food products**
ISO 7952: 1994	Fruits, vegetables and derived products – Determination of copper content – Method using flame atomic absorption spectrometry
ISO 9167-2: 1994	Rapeseed – Determination of glucosinolates content – Part 2; Method using X-ray fluorescence spectrometry
ISO 11051: 1994	Durum wheat (*Triticum durum* Desf.) – Specification
ISO 11294: 1994	Roasted ground coffee – Determination of moisture content – Method by determination of loss in mass at 103°C (Routine method)
ISO 11817: 1994	Roasted ground coffee – Determination of moisture content – Karl Fischer method (Reference method)
TC 45	**Rubber and rubber products**
ISO 5771: 1994	Rubber hose and hose assemblies for transferring anhydrous ammonia – Specification
ISO 6803: 1994	Rubber or plastics hoses and hose assemblies – Hydraulic-pressure impulse test without flexing
ISO 6605: 1994	Rubber hoses and hose assemblies for underground mining – Wire-reinforced
	hydraulic types for coal mining – Specificaiton
ISO 8789: 1994	Rubber hoses and hose assemblies for liquefied petroleum gas in motor vehicles – Specification
TC 46	**Information and documentation**
ISO 12083: 1994	Information and documentation – Electronic manuscript preparation and markup
TC 61	**Plastics**
ISO 308: 1994	Plastics – Phenolic moulding materials – Determination of acetone-solubre matter (apparent resin content of material in the unmoulded state)
ISO 1597: 1994	Plastics – Unplasticized cellulose acetate – Determination of acetic acid yeild
ISO 4892-3: 1994	Plastics – Methods of exposure to laboratory light sources – Part 3; Fluorescent UV lamps
TC 139	**Plastics pipes, fittings and valves for the transport of fluids**
ISO 4440-1: 1994	Thermoplastics pipes and fittings – Determination of melt mass-flow rate – Part 1: Test method
ISO 4440-2: 1994	Thermoplastics pipes and fittings – Determination of melt mass-flow rate – Part 2; Test conditions
TC 172	**Optics and optical instruments**
ISO 8597: 1994	Optics and optical instruments – Visual acuity testing – Method of correlating optotypes
ISO 11380: 1994	Optics and optical instruments – Ophthalmic optics – Formers

The following International Standards are confirmed for a 5-year period.

TC 5	**Ferrous metal pipes and metallic fittings**
ISO 3545-1: 1989	
ISO 3545-2: 1989	
ISO 3545-3: 1989	
TC 27	**Solid mineral fuels**
ISO 9411-1: 1994	Solid mineral fuels – Mechanical sampling from moving streams – Part 1: Coal
TC 28	**Petroleum products and lubricants**
ISO6617: 1994	Petroleum-based lubricating oils – Aging characteristics – Determination of change in Conradson carbon residue after oxidation
ISO 7507-1: 1993**	Petroleum and liquid petroleum products – Calibration of vertical cylindrical tanks – Part 1: Strapping method
TC 34	**Agricultural food products**
ISO 8294: 1994	Animal and vegetable fats and oils – Determination of copper, iron and nickel contents – Graphite furnace atomic absorption method
ISO 12193: 1994	Animal and vegetable fats and oils – Determination of lead content – Graphite furnace atomic absorption method
TC 43	**Rubber and rubber products**
ISO 6446: 1994	Rubber products – Bridge bearings – Specification for rubber materials
ISO 7617-1: 1994	Plastics -coated fabrics for upholstery – Part 1: Specification for PVC-coated knitted fabrics
ISO 7617-2: 1994	Plastics-coated fabrics for upholstery – Part 2: Specification for PVC-coated woven fabrics
TC 61	**Plastics**
ISO 1622-1: 1994	Plastics – Polystyrene (PS) moulding and extrusion materials – Part 1: Designation system and basis for specifications
ISO 2580-2: 1994	Plastics – Acrylonitrite/butadiene/stryene (ABS) moulding and extrusion materials – Part 2: Preparation of test specimens and determination of properties
ISO 2897-2: 1994	Plastics – Impact-resistant polystyrene (PS-1) moulding and extrusion materials – Part 2: Preparation of test speciments and determination of properties

Conferences

3rd International Symposium on Functional Dyes
UC Santa Cruz, California
16–21 July 1995

IUPAC SPONSORED

The 3rd International Symposium on Functional Dyes (Functional Dyes '95) will be held in the University of California Santa Cruz (UCSC), on 16–21 July. The objective of this symposium will be to bring together scientists and engineers from both academic and industrial laboratories to discuss recent developments in all aspects of functional dyes and their applications. By functional dyes we mean organic molecules which, besides having colour, have interesting functional properties such as luminescence, non-linear optical constants, etc., which make them useful for a variety of applications, i.e. these are the molecules which play an essential role when one wants to do something with light. Thus the topics being addressed are highly interdisciplinary and it is expected that there will be a cross fertilization of ideas and inspiration between scientists and engineers of various backgrounds.

The official language of the conference is English and the Symposium will feature five plenary lectures, over twenty invited lecturers, many oral presentations and/or posters. It will be concerned with the design of functional dye materials, including computer aided design, their synthesis and characterization in terms of structure, reactivity and function. The application of interest range from information display and recording, energy conservation and non-linear optical devices, and applications in biotechnology.

The Third International Symposium will be the first of this series to be sponsored by IUPAC and the emphasis will be on novel functional materials, functional dyes in biological applications and computer aided design of the functional dyes.

The following is a list of the Plenary Lectures and the lecture title:

- Professor Norbert Hampp (University of München, Germany) Functional Dyes from Nature: Potentials for Technical Applications;
- Professor Masahiro Iric (Kyushu University, Japan) Photochromic Diarylethenes for Photonic Devices;
- Dr George D. Pruvis, III (CAChe Scientific, USA) Computer Simulation of Dye Absorption for Bench Chemists;
- Professor Emanuel Vogel (Institute of Organic Chemistry, Germany) Porphyrinoid Macrocycles: A cornucopia of Novel Chromophores;
- Professor Fred Wudl (University of Cal., at Santa Barbara, USA);
- Photoinduced Electron transfer from Conjugated Polymers to Functionalized Buckminsterfullerene: Interactions Between Two Unusual Dyes.

UCSC is one of the most beautiful of the University of California campuses. Located on 2000 acres of what was formerly the Cowell Ranch, it overlooks Monterey Bay and the Pacific Ocean to the south-west. It is surrounded by unspoiled redwoods and meadows and enjoys cool, misty mornings and bright afternoons with the average summer temperature in the mid-20 °C.

The registration fee is USD300 for academic personnel, USD400 for industrial personnel and USD50 for students. The University housing is available in a 5 day package of USD425 including 3 meals a day.

For further information or the 2nd Circular please contact: Dr Kay Kanazawa, General Secretary of the Symposium, IBM Research Division, Almaden Research Center, 650 Harry Road K42/803, San Jose, CA 95/20–6099, USA. Fax (408) 927–2213. E-mail kanazawa @almaden. ibm.com.

12th International Symposium on Plasma Chemistry. ISPC 12
21–25 August 1995
Minneapolis, Minnesota, USA

IUPAC SPONSORED

The International Symposium on Plasma Chemistry (ISPC) is held biennially at various host institutions around the world. The ISPC is the main international plasma chemistry symposium, encompassing the whole area of plasma chemistry, including high-pressure thermal plasmas, low-pressure non-equilibrium plasmas and high-pressure non-equilibrium dis-

Minneapolis and the campus of the University of Minnesota along the Mississippi river.

charges. The wide range of topics discussed at these symposia make them ideally suited for the exchange of ideas between international scientists from a range of disciplines. Accordingly, past conferences have attracted a mix of participants from academia and various industries, from many countries (35 at the last symposium), both world renowned scientists and students.

The planned symposium will have plenary sessions for all participants and parallel topical sessions, including poster sessions, for the more expert. The topics to be discussed include:

General Sessions
- Characterization of the properties of plasmas;
- Fundamentals of plasma-particle interactions;
- Fundamentals of plasma-surface interactions.

Special Sessions
- High-pressure non-equilibrium plasmas;
- Plasma chemistry for environmental applications;
- Controls in plasma processing;
- Large area plasma sources.

Sessions on Specific Applications
- Plasma, etching for microelectronic and micromechanical components;
- Plasma polymerization;
- Plasma synthesis;
- Plasma CVD;
- Plasma spraying;
- Plasma surface modification;
- Plasma metallurgical processing.

There will be eight invited plenary lectures of a general nature and approximately 20 topical invited lectures on recent accomplishments. A Plasma Chemistry Prize will be awarded to the contributed paper offering the most noteworthy and original research result.

The meeting will be held on the main campus of the University of Minnesota, on the banks of the Mississippi river. To corroborate the objectives of the symposium, there will be a Summer School on Plasma Chemistry held before the symposium (17–19 August 1995) and a workshop on Industrial Applications of Plasma Chemistry following the symposium (25–26 August 1995).

The conference language is English. The registration fee is USD275 for those who register before 15 June 1995, and USD325 for registration after this date. The registration fee for a student is USD75. There are several hotels within walking distance from the conference site, offering rooms for USD60–85 and dormitory housing is available for USD35 per person per night (including breakfast).

Minneapolis offers many cultural and recreational opportunities, ranging from visits to numerous theatres, concerts and museums, to water sports at one of the many lakes for which the state of Minnesota is famous.

Further information is available from: Conference Office, ISPC-12 c/o Catherine Ploetz, University of Minnesota, 218 Nolte Center, 315 Pillsbury Drive S.E., Minneapolis, MN 55455–0139, USA, Tel.: (1) 612–626–2259, Fax: (1) 612–626–1632, E-mail: ISPC12@PDCS.CEE.UMN.EDU

Ninth International Conference on Liquid and Amorphous Metals (LAM-9)
27 August – 1 September 1995
Chicago, Illinois, USA

IUPAC
SPONSORED

The tradition of these conferences strongly encourages the participation of junior researchers and graduate students. The meeting will include single sessions of invited and selected contributed papers, as well as poster displays. Visits to the Advanced Photon Source and the Intense Pulsed Neutron Source at Argonne National Laboratory will be arranged. A technical exhibit featuring a wide range of advanced instruments, computer hardware and software, together with publications, will accompany the meeting.

The following topics will be covered:
- Liquid and amorphous metals and alloys;
- Metal-nonmetal transitions;
- Clusters;
- Composite materials;
- Quasicrystals;
- Metal/molten salt mixtures.

Stouffer Riviere Hotel, Chicago.

Other subjects for discussion will include, the determination of atomic structure by X-ray, neutron and electron diffraction. Together with studies of dynamics and electrical transport properties; also included will be work on magnetic, optical and thermodynamic properties. Both experimental and theoretical, including computational, approaches to these problems will be addressed. Results obtained from new sources, taking full advantage of recently commissioned synchrotron and both pulsed neutron and continuous neutron sources, will be emphasized. High-lighted topics include new structural materials and applications in energy conversion, electronics, waste disposal and electro-optics.

The conference will be held in the Stouffer Riviere Hotel, Chicago, Illinois, which overlooks the Chicago River.

Chicago is one of the great cities of the world, and one of the most beautiful in the United States featuring works by some of the greatest 20th century architects, including Burnham, Sullivan, Wright and van der Rohe. Public sculptures by Picasso, Chagall, Miro, Calder and Oldenburg grace the city center. Chicago has several outstanding museums and art galleries, including the Art Institute of Chicago. Many musical festivals run throughout the summer and early autumn, ranging from the well known Jazz/Blues festival in Grant park to the classical series in Ravinia Park.

Inquiries dealing with the scientific programme should be addressed to: Prof. John van Zytveld, Physics Department, Calvin College, 3201 Burton SE, Grand Rapids, MI 49546, USA, Tel: +1616 9576340, Fax: +1616 9576501.

Inquiries dealing with the technical exhibit should be addressed to: Mr Hans J. Luedi, President, Midwest Vacuum Inc., 201 E. Ogden Avenue, Suite 15, Hinsdale, IL 60521, USA, Tel: +1708 3235399, Fax: +1708 3232142.

Medicinal Chemistry 3–8 September 1995 Tokyo, Japan

IUPAC
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The Asian Federation for Medicinal Chemistry (AFMC) has organized a large international symposium on Medicinal Chemistry to he held in Tokyo, Japan, on 3–8 September 1995, at the Keio Plaza Hotel, Tokyo. AIMECS 95.

The AFMC International Medicinal Chemistry Symposium (AIMECS 95) will be held at the Keio Plaza Hotel, Tokyo. The object of this meeting is the presentation of recent results, discussion of trends, and an exchange of ideas about medicinal chemistry for the discovery, development and production of new pharmaceuticals. It is estimated that more than twelve hundred participants from over fifty countries may well attend this symposium.

AIMECS 95

AFMC International Medicinal Chemistry Symposium

This is the first world-wide symposium on medicinal chemistry linking Asian countries (AFMC), European countries (European Federation for Medicinal Chemistry) and North American (Division of Medicinal Chemistry, American Chemical Society) organizations. This landmark event will strive to strengthen cooperation between industry, government and universities throughout the world.

AIMECS 95 is sponsored by IUPAC and is supported by the Japan Health Sciences Foundation and the Research Foundation for Pharmaceutical Sciences. In addition, it is expected that there will be additional support from the Ministry of Health and Welfare, Japan.

The symposium will have 13 sessions around which the plenary and invited lectures, and poster sessions will include discussion of the following topics:

- **chemistry for pharmaceuticals**
  natural products;
  new synthetic routes;
  lead optimization in drug design;
  industrial synthetic routes;
  fermentation and biotechnology in the pharmaceutical industry.
- **Traditional medicine**
- **Molecular diversity** (organized by Division of Medicinal Chemistry, American Chemical Society).
- **Computer-assisted drug design**
  lead discovery;
  3D structure – activity relationships;
  protein structure and modelling;
  2D/3D databases.
- **Endogenous substances**
  prostaglandins;
  nitric oxide;
  peptides;
  lipids;
- **Receptors: structure and function**
  receptor structure;
  signal transduction;
  ion channels and drugs;
  transporters;
- **Enzyme inhibitors**
- **Drug metabolism and toxicology**
- **Drug delivery**
  prodrugs;

targeting;
polymer conjugates;

- **Glycobiology and glycotechnology**
- **Biomaterials, biomimetics and medicinal biotechnology**

chemistry and biology of molecular adhesion;
antibody engineering;
gene function and drug design;
cytokines, cytokine receptors, growth factors as drug sources;

- **Regulatory affairs**
- **Topics from pharmaceutical industry**

Eight plenary lectures have been organized. Topics for discussion will include; a new method for the design of candidate structures from pharmacophoric hypotheses, targeting the delivery of prostanoids and bioactive proteins, functional analysis of neuropeptide and glutamate receptors by drug-based molecular approaches, biologically active microbial metabolites, organic synthesis for organic and bioorganic targets, prospects for pharmaceuticals from marine organisms, anti-cancer taxoids and cytokine receptors as a new tool for the therapy of inflammation.

In addition, more than 40 invited lectures will hopefully present a clear and accurate description of the state of their activities towards the discovery and development of pharmaceuticals, including interdisciplinary research comprising molecular design, chemistry, biochemistry, molecular biology, pharmacology and drug delivery. The official language of the conference will be English.

Registration fees for participants are JPY60 000 (Japanese yen) for delegates (IUPAC members are entitled to a reduction of 10%), JPY20 000 for students and JPY10 000 for accompanying persons. On and after 1 June 1995, registration fees will be JPY70 000 for participants and JPY25 000 for students.

The weather in Tokyo during the symposium will probably be mild, with temperatures in the lower 20's Celsius, and with occasional rainfall.

For further information please contact: Professor Shiro Ikegami, Secretary General, AIMECS 95, c/o Faculty of Pharmaceutical Sciences, Teikyo University, Sagamiko, Kanagawa 199 01, Japan, Tel: +81 426 85 0161, Fax: +81 426 85 1870, Telex: 2862552 TKPLIBJ.

Third International Symposium on Bio-organic Chemistry (ISBOC 3) 17–23 September 1995 Dagomys, Russia

IUPAC
SPONSORED

The 3rd International symposium on Bioorganic Chemistry (ISBOC) will be held in Dagomys, Russia, on 17–23 September 1995.

Chairman of the 3rd ISBOC Symposium, Professor Vadim T. Ivanov.

The purpose of the symposium is to bring together researchers from all over the world to share their ideas and to learn from each other about their advances to this branch of chemistry. The symposium will cover the areas related to the organic chemistry of biological processes. These include:

- Chemical Design of Bioactive Molecules;
- Structure as a Key to the Mechanism of Activity;
- Bioorganic Chemistry of Enzyme Catalysis;
- Mechanisms of Biomolecular Recognition;
- Chemical Aspects of Gene Expression.

The symposium is expected to demonstrate the various innovations in the above fields combined with cooperation at international levels.

There will be a number of plenary lectures, together with feature section lectures and poster sessions. It is hoped that the speakers will summarize the current contributions and the different concerns of the community and suggest how the subject will move in the near future.

The official working language of the symposium will be English.

The registration fee for full participants is USD400 if paid before 17 May 1995 and USD475 if paid after this date. For a student, the registration fee is USD175 and for an accompanying person it is USD200. For scientists from countries in Eastern Europe and those countries which made up the former Soviet Union, the registration fee is USD175. there is a charge of USD50 for the Conference banquet.

The symposium site is the Dagomys hotel complex near the city of Sochi on the Black Sea coast. The area has a mild climate, with a rich sub-tropical vegetation. The average temperature in summer is 25 °C and the sea temperature at this time is never below 20 °C. The countryside around the conference site is rich in natural attractions, with caves, lakes and tea plantations.

For additional information, please contact: Secretariat, 3rd ISBOC, Dr Victor V. Demin, Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Ul. Miklukho Maklaya, 16/10, 117871 Moscow V437, Russia, Tel: +7 95 335 15 11 and +7 95 330 63 38, Fax: +7 95 310 70 07.

11th International Conference on Organic Synthesis (ICOS-11) 30 June – 4 July 1996 Amsterdam, the Netherlands

IUPAC SPONSORED

The 11th international conference on organic synthesis will be held in Amsterdam at the end of June in 1996. The conference will emphasize all important aspects of the creative science of modern organic synthesis.

The conference programme will include plenary lectures, section lectures, contributed oral papers and poster presentations. The following topics will be highlighted: (1) New synthetic methods;(2) Stereoselective synthesis; (3) Metal-mediated synthesis; (4) Target organic synthesis.

In addition, there will be a mini-symposium devoted to Synthesis Directed to Complex Medicinal Agents.

The conference will be held at the RAI International Exhibition and Congress Centre, Amsterdam. The conference language will be English.

Amsterdam, the capital of The Netherlands, is a historic city of great beauty and character, providing opportunities for a wide variety of activities to the visitor. Its charming old canal houses, still in active use, make it a veritable living museum. The extensive network of canals with their associated bridges has earned Amsterdam the name of 'the Venice of the North'. The city is a rich cultural centre, being the residence of the famous Concertgebouw Orchestra and housing many fine museums, such as the Rijksmuseum, containing works by Rembrandt, and the Van Gogh Museum.

Details: Scientific Secretariat, Dr H. Hiemstra, Laboratory of Organic Chemistry, University of Amsterdam, Nieuwe Achtergracht 129, 1018 WS Amsterdam, the Netherlands, Tel +31 205255941, Fax +31 205255670, E-mail: henkh@org.chem.uva.nl, Conference Secretariat, Van Namem & Westerlaken, Congress Organization Services, PO Box 1558, 6501 BN Nijmegen, The Netherlands, Tel: +31 80 234471, Fax: +31 80 601159.

Conference Calendar

1995

Macrocyclic chemistry

2–7 July
20th International Symposium on Macrocyclic Chemistry. Jerusalem, Israel.
Prof. D. Meyerstein, Chemistry Department, Ben-Gurion University of the Negev, P.O.B. 653, Beer-Sheva 84105, Israel. Tel: +972 (7) 461238. Fax: +972 (7) 237682

Polymer morphology and electrical properties

5–7 July
International Symposium on Polymer Morphology and Electrical Properties. Lodz, Poland.
Prof. A. Galeski, Centre of Molecular & Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, 90–363 Lodz, Poland. Tel: +48 (42) 818952 or 815761. Fax: +48 (42) 847126 or 815483. E-mail: julanski@lodzl.p.lodz.pl.

Analytical chemistry

9–15 July
SAC 95: International Conference on Analytical Chemistry. Hull, UK.
Prof. A. Townshend, School of Chemistry, University of Hull, Hull HU6 7RX, UK. Tel: +44 (482) 465027. Fax: +44 (482) 466410.

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Toxicology and clinical chemistry of metals

10–13 July
5th COMTOX Symposium on Toxicology and Clinical Chemistry of Metals. Vancouver, BC, Canada.
Prof. F. W. Sunderman, Jr., Departments of Laboratory Medicine and Pharmacology, University of Connecticut Medical School, Post Office Box 1292, Farmington, CT 06034-1292, USA. Tel: +1 (203) 792328. Fax: +1 (203) 6792154.

High swelling gels

10–14 July
36th Microsymposium on Macromolecules – High Swelling Gels. Prague, Czech Republic.
P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague 6, Czech Republic. Tel: +42 (2) 360341. Fax: +42 (2) 367981. E-mail: sympo@imc.cas.cz.

Functional dyes

16–21 July
3rd International Symposium on Functional Dyes (Functional Dye '95). Santa Cruz, California, USA.
Dr Kay Kanazawa, IBM Research Division, Almaden Research Center, 650 Harry Road K42/803., San Jose, CA 95120-6099, USA. Fax: +1 (408) 9272213.

Heteroatom chemistry

30 July – 4 August
4th International Conference on Heteroatom Chemistry. Seoul, Korea.
Prof. Kyongtae Kim, Secretary General, ICHAC-4, Department of Chemistry, Seoul National University, Seoul 151-742, Korea. Tel: +82 (2) 8806636. Fax: +82 (2) 8748858.

Chemistry in Africa

30 July – 4 August
6th International Conference on Chemistry in Africa. Accra, Ghana.
Prof. I. Addae-Mensah, Chemistry Department, University of Ghana, Legon/Accra, Ghana. Fax: +223 (21) 777098.

Novel aromatic compounds

31 July – 4 August
8th International Symposium on Novel Aromatic Compounds (ISNA-8). Braunschweig, Germany.
Prof. H. Hopf, Institut für Organische Chemie, Technische Universität, Hagenring 30, D-38106 Braunschweig, Germany. Tel: +49 (531) 391 5255. Fax: +49 (531) 391 5388

IUPAC General Assembly

4–11 August
38th IUPAC General Assembly. Guildford, Surrey, UK.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion

Organometallic chemistry directed toward organic synthesis

6–10 August
8th IUPAC Symposium on Organometallic Chemistry directed toward Organic Synthesis (OMCOS-8). Santa Barbara, California, USA.
Prof. B. H. Lipshutz, Department of Chemistry, University of California, Santa Barbara, California 93106–9510, USA. Tel: +1 (805) 8933072. Fax: +1 (805) 8937287. E-mail hr03conf@ucsbvm.ucsb.edu.

Heterocyclic chemistry

6–11 August
15th International Congress of Heterocyclic Chemistry. Taipei, Taiwan, China.
Prof. Chin-Kang Sha, Department of Chemistry, National Tsing Hua University, Hsinchu 300, Taiwan, China. Tel: +86 (35) 722427. Fax: +86 (35) 725870. E-mail: cksha@chem.nthu.edu.tw.

35th IUPAC Congress

14–19 August
35th IUPAC Congress. Istanbul, Turkey.
Prof. A. Riza Berkem, Halasgargazi Cad. No. 53, D. 8, 80230 Harbiye, Istanbul, Turkey. Tel: +90 (212) 2407331. Fax: +90 (212) 2317037.

Plasma chemistry

21–25 August
12th International Symposium on Plasma Chemistry. Minnesota, Minneapolis, USA.
ISPC-12, c/o Catherine Ploetz, 218 Nolte Center, University of Minnesota, 315 Pillsbury Drive SE, Minneapolis, MN 55455, USA. Tel: +1 (612) 6262259. Fax: +1 (612) 6261632. E-mail: ispc12@pdcs.cee.umn.edu

Spectroscopy

27 August – 1 September
29th Colloguium Spectroscopicum Internationale. Leipzig, Germany.
CSI XXIX Secretariat, Gesellschaft Deutscher Chemiker, Abt. Tagungen, Postfach 90 04 40, D-60444 Frankfurt am Main, Germany. Tel: +49 (69) 7917358. Fax: +49 (69) 7917475.

Liquid and amorphous metals

27 August – 1 September
9th International Conference on Liquid and Amorphous Metals. Chicago, USA.
Drs. Saboungi and Price, Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA. Tel: +1 (708) 252 4341 (M.-L. Saboungi), +1 (708) 252 5475 (D.L.Price). Fax: +1 (708) 252 7777 (both)

Industry – education initiatives in chemistry

28 August – 2 September
International Symposium on Industry – Education Initiatives in Chemistry. York, UK.
Dr J. F. Gibson, The Royal Society of Chemistry, Burlington House, Piccadilly, London WIV OBN, UK. Tel: +44 (0)71 437 8656. Fax +44 (0)71 734 1227.

Solution chemistry

29 August – 2 September
24th International Conference on Solution Chemistry. Lisbon, Portugal.
Prof. C. A. N. Viana, Instituto Bento da Rocha Cabral, F.C.U.L., Calçada Bento da Rocha Cabral, 1200 Lisboa, Portugal. Tel: +351 (1) 3859628/608823. Fax: +351 (1) 7977837.

Medicinal chemistry

3–8 September
AFMC International Medicinal Chemistry Symposium (AIMECS 95). Tokyo, Japan.
Prof. S. Ikegami, Secretary General, AIMECS 95, c/o Faculty of Pharmaceutical Sciences, Teikyo University, Sagamiko, Kanagawa 199–01, Japan. Tel: +81 (426) 850161. Fax: +81 (426) 851870.

Ionic polymerization

4–8 September
1st International Symposium on Ionic Polymerization. Istanbul, Turkey.
IUPAC International Symposium on Ionic Polymerization, c/o Prof. Y. Yagci, Istanbul Technical University, Faculty of Science, Department of Chemistry, Maslak 80626, Istanbul, Turkey. Tel: +90 (212) 285 32 41. Fax: +90 (212) 285 63 86.
E-mail: Feyusuf@TRITU

Applications of the mössbauer effect

10–16 September
International Conference on the Applications of the Mössbauer Effect (ICAME-95). Rimini, Italy.
Prof. I. Ortalli, ICAME-95, University of Parma, Istituto di Scienze Fisiche, Via M. D'Azeglio 85, I-43100 Parma, Italy. Tel: +39 (521) 902231. Fax: +39 (521) 236508. E-mail: ICAME95@ipruniv.cce.unipr.it

Bioorganic chemistry

17–23 September
3rd International Symposium on Bioorganic Chemistry. Dagomys, Sochi region of Black Sea Coast, Russia.
Dr V. V. Demin, Shemyakin – Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Ul. Miklukho-Maklaya, 16/10, 117871 Moscow V-437, Russia. Tel: +7 (095) 3351511, 330 6338, 3302800. Fax: +7 (095) 3107007.

Chromatography of polymers

18–22 September.
International Symposium on Chromatography of Polymers and Related Substances. Bratislava, Slovakia.
Dr D. Berek, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, Sk-842 36 Bratislava, Slovakia. Tel: +42 (7) 3782306. Fax: +42 (7) 375923.

Assessment carcinogenic risk

17–20 October
International Symposium on the Assessment of Respiratory Carcinogenic Risk from Occupational Exposure to Inorganic Substances. Luxembourg.
Dr J. H. Duffus, Director, The Edinburgh Centre for Toxicology, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS, Scotland. Tel: +44 (131) 4513456. Fax: +44 (131) 4513017.

Environmental catalysis

25–27 October
2nd International Forum on Environmental Catalysis. Tokyo, Japan.
Prof. Makoto Misono, Department of Applied Chemistry, Faculty of Engineering, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan. Tel: +81 (3) 3812 2111 Ext. 7272. Fax: +81 (3) 5802 2949.

Soil chemistry and ecosystem health

28 October
Workshop on Soil Chemistry and Ecosystem Health. St. Louis, MO, USA.
Prof. P. M. Huang, Dept of Soil Science, University of Saskatchewan, Saskatoon, Saskatchewan S7N OWO, Canada. Tel: +1 (306) 9666823. Fax: +1 (306) 9666881.

Automation and new technology in clinical laboratory

2–4 November 1995
6th International Congress on Automation and New Technology in Clinical Laboratory. Sitges, Barcelona, Spain.
Dr F. Javier Gella, BioSystems, S.A., Costa Brava 30, 08030 Barcelona, Spain. Tel: +34 (3) 3110811. Fax: +34 (3) 3117609.

1996

Free-radical polymerization

26–31 May
2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism. Santa Margherita Ligure, Genoa, Italy.
Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy. Tel: +39 (79) 229556. Fax: +39 (79) 229559

Mycotoxins and phycotoxins

27–31 May
9th International Symposiums on Mycotoxins and Phycotoxins. Rome, Italy.
Dr Marina Miraglia, Instituto Superiore Sanità, Food Department, Viale Regina Elena, 299, I-00161 Rome, Italy. Tel: +39 (6) 4990 x 377. Fax +39 (6) 4451767.

Organic synthesis

30 June – 4 July
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Conference Secretariat ICOS - 11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel: +31 (80) 234471. Fax: +31 (80) 601159.

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.
Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

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Front cover: Complex calculations need not be undertaken solely on Si-based technology.

International Union of Pure and Applied Chemistry

Molecules as Computers

Prof. Leonard Adleman is at the Department of Computer Science in the University of Southern California, and is well known for his work in the development of computer security systems. He is the 'A' in the RSA (Rivest–Shamir–Adleman) encryption system. He is also someone who is active in the development of new computer technology, for example, he has demonstrated a new type of computer program designed to reproduce itself surreptitiously. Prof. Adleman is someone who looks at computers in biological terms, indeed, he was the first to coin the phrase 'computer virus'.

Perhaps, it is this ability to look at computers from a broader perspective, with the eyes of the child who beheld the emperor's new cloths, that has allowed Adleman to achieve what many chemists and computer scientists think is one of the most exciting advances in the development of new computers. In a recent issue of *Science* (**266**, 1021 (1994)), Adleman used the tools of molecular biology and solution chemistry to solve a problem in topology (the field of mathematics which deals with the properties of surfaces). A small graph was encoded in molecules of DNA and the operations of the computation were performed with standard protocols and enzymes. Thereby demonstrating the feasibility of carrying out computations at the molecular level.

Hundreds of difficult practical computational problems, including optimal shop scheduling, the longest path in a graph and Boolean logic satisfaction, can be translated into a classic form known as a directed Hamiltonian problem. Imagine for the moment a graph in two dimensions consisting of n points or vertices (Fig. 1). A path through such a graph is said to be Hamiltonian if it visits each vertex once and only once. Finding such paths for complex graphs is not at all easy. Many commercial algorithms, applied even to modest sized graphs, require an impractical amount of computer time to render a decision. This is because the Hamiltonian path problem has been proven to be NP-complete and all known algorithms for this problem have exponential worst-case complexity.

Problems in computer science are ranked by their computational difficulty. There are the easy polynomial problems (algorithms whose running time is bounded by a polynomial function), the more difficult exponential problems (problems where the running time of the algorithm is bounded by an exponential power law), and finally the universal machine problems (open boundary dependence).

A problem is referred to as intractable if there is no polynomial time algorithm that can solve it. Consider the following example, if an $O(n^2)$ algorithm takes one microsecond to solve a problem of size 10, then it will take 100 microseconds to solve a problem of size 100. However, if an $O(2^n)$ algorithm takes one microsecond to solve a problem of size 10, then it will take 3.9×10^{11} centuries to solve a problem of size 100!

The directed Hamiltonian problem is in the complexity class of computational problems known as non-deterministic polynomial time (NP). Such a problem can have its answer checked in polynomial time. Indeed, the Hamiltonian path problem is a special case of an NP problem, i.e. NP-complete. Many important problems are NP-complete, to make them practical computationally, their sizes are limited and acceptable approximations are made in order to offset numerical precision for execution time.

Adleman has approached the Hamiltonian path problem in a biological context where each vertex and edge in his graph can be represented by a short oligonucleotide sequence. An oligonucleotide is a synthetic single stranded DNA molecule made with a chosen sequence of nucleotide bases. Adleman has shown that the binding together of chosen oligonucleotides representing vertices results in DNA molecules that encode the solution to a particular Hamiltonian path problem. Adleman further describes how to choose the right oligonucleotides to 'input' a problem into his method, and how to isolate and interpret the DNA molecules that represent solutions which are the 'output' of his computational method. The following non-deterministic algorithm solves the directed Hamiltonian path problem:

Step 1: Generate random paths through the graph.
Step 2: Keep only those paths which start and end with particular vertices.
Step 3: If the graph has n vertices, keep only those paths that enter exactly n vertices.
Step 4: Keep only those paths which enter all of the vertices of the graph at least once.
Step 5: If any path remains, say Yes, otherwise say No.

The figure shows the example directed graph. The problem is to find a route which visits each vertex only

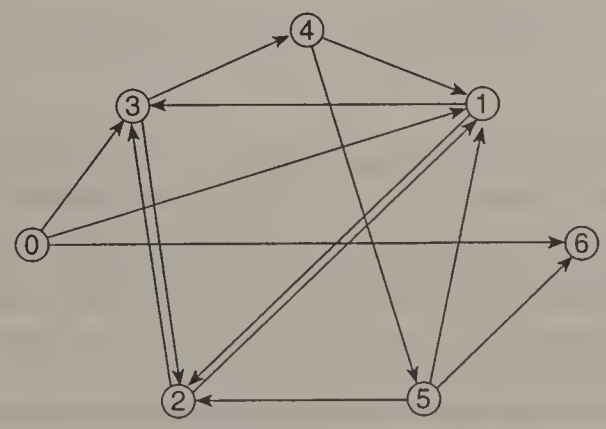

Figure 1. Directed graph. When $v_{in} = 0$ and $v_{out} = 6$, a unique Hamiltonian path exists: 0⇒1, 1⇒2, 2⇒3, 3⇒4, 4⇒5, 5⇒6.

once starting with $v_{in} = 0$ and ending with $v_{out} = 6$. To implement Step one of the algorithm, each vertex i in a seven-point graph was associated with a random 20-mer sequence of DNA denoted O_i. For each edge $i \Rightarrow j$ in the graph, an oligonucleotide $O_{i \Rightarrow j}$ was created that was the 3′ 10-mer of O_i (unless $i = 0$, in which case it was all of O_i) followed by the 5′ 10-mer of O_j (unless $j = 6$, in which case it was all of O_j). Notice that this construction preserves edge orientation. For example, $O_{2 \Rightarrow 3}$ will not be the same as $O_{3 \Rightarrow 2}$. The 20-mer oligonucleotide with the sequence which is Watson–Crick complementary to O_i is denoted O_{i*}.

For each vertex i in the graph (except $i = 0$ and $i = 6$) and for each edge $i \Rightarrow j$ in the graph, 50 pmol of O_{i*} and 50 pmol of $O_{i \Rightarrow j}$, respectively, were mixed together in a single ligation reaction. The O_{i*} oligonucleotides served as splints to bring oligonucleotides associated with compatible edges together for ligation (Fig. 2). Hence the ligation resulted in the formation of DNA molecules encoding random paths through the graph.

The scale of this ligation reaction far exceeds what is required to encode the graph under consideration. For each edge in the graph under consideration, $\approx 3 \times 10^{13}$ copies of the associated oligonucleotides were added to the ligation reaction. hence, it is likely that many DNA molecules encoding the Hamiltonian path were created. In theory, the creation of a single such molecule would be sufficient. As a result, for this graph quantities of oligonucleotides less than an attomole would probably have been sufficient. Alternatively, a much larger graph could have been encoded with the picomole quantities used here.

To implement Step two of the molecular algorithm, the products of Step one were amplified using the polymerase chain reaction (PCR) using primers O_0 and O_{6*}. Thus, only those molecules encoding paths that begin with vertex 0 and end with vertex six were amplified. Step three required the separation on an agarose gel of the products from Step 2. The 140-base-pair band, corresponding to double stranded DNA encoding paths entering exactly seven vertices, was extracted from the gel. This product was re-amplified to enhance purity.

To implement Step 4, the product of Step 3 was affinity-purified with a biotin-avidin magnetic bead system. Single stranded DNA was first generated from the double stranded DNA of Step 3 and then incubated with O_{1*} conjugated to magnetic beads. Only those single stranded DNA molecules that contained the sequence O_1, and hence encoded paths that enter vertex 1 at least once, annealed to the bound O_{1*} and were retained. This process was repeated successively with O_{2*}, O_{3*}, O_{4*} and O_{5*}. To implement Step 5, the product of Step 4 was amplified by PCR and run on a gel. The result of this 'calculation' may then be extracted and its sequence determined – yielding the desired Hamiltonian path.

This 'computation' required 7 days of laboratory work. Step four requiring a full day at the bench. In essence, Adleman is using the enormous parallelism of solution-phase chemistry to solve a hard computational problem.

What is the potential of this new-type of computer? A typical desk-top computer can execute 10^6 operations per second and the fastest supercomputers can undertake 10^{12} operations per second. If we assume that the ligation reaction of two DNA molecules is considered as a single operation, and if it is further assumed that half of the $\approx 4 \times 10^{14}$ edge oligonucleotides in Step 1 are ligated, then during Step 1 $\approx 10^{14}$ operations were executed. This number could readily be scaled up by, for example, increasing the concentrations of the ligating oligomers. Indeed, 10^{20} operations per second seems plausible. Furthermore, hydrolysis of a single molecule of ATP to ADP provides the Gibbs free energy, of order 33 kJ mole^{-1} for one ligation reaction; hence there are in principle 2×10^{19} such ligation operations for each available joule. This is a particularly energy efficient process considering that the theoretical limit (2nd Law of Thermodynamics) is 34×10^{19} irreversible operations per joule. Finally, storing information in a molecule of DNA allows for an information density of about 1 bit per cubic nanometer, a dramatic improvement over existing storage media such as video-tapes, which store information at a density of ≈ 1 bit per 10^{12} cubic nanometers.

In the future, it will be hoped that materials science will provide improved techniques for the manipulation and separation of very small quantities of macromolecules. Research in chemistry may allow for the development of synthetic designer-enzymes. One can imagine the eventual emergence of a general purpose molecular computer, being nothing more substantial that a single macromolecule conjugated to a ribosome-like collection of enzymes which act upon it. The whole assembly bathed in a solution from which it extracts the chemical energy necessary to function.

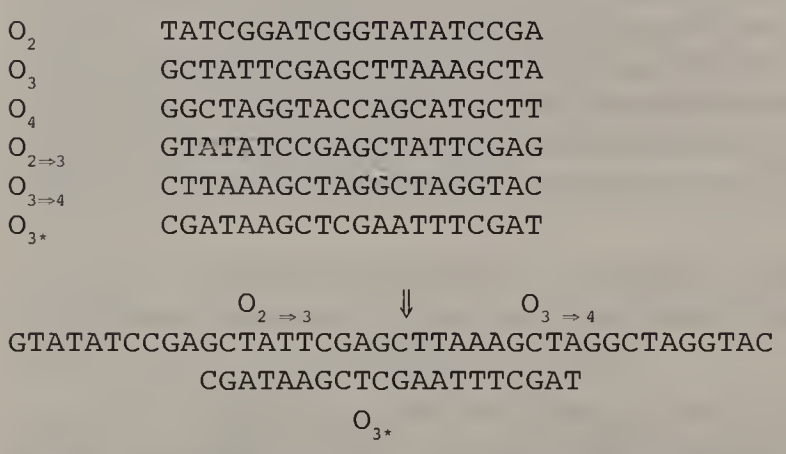

Figure 2. Encoding a graph in DNA. For each vertex *i* in the graph, a random 20-mer oligonucleotide (shown here are O_2, O_3 and O_4, for vertices 2, 3 and 4, respectively). For edges $i \Rightarrow j$ in the graph, an oligonucleotide $O_{i \Rightarrow j}$ is derived from the 3' 10-mer of O_i and from the 5' 10-mer of O_j (shown as $O_{2 \Rightarrow 3}$ for edge $2 \Rightarrow 3$ and $O_{3 \Rightarrow 4}$ for edge $3 \Rightarrow 4$). For each vertex *i* in the graph, O_{i*} is the Crick-Watson complement of O_i (shown as O_{3*}, which is the Crick–Watson complement of O_3). O_{3*} serves as a splint to assist in the binding of $O_{2 \Rightarrow 3}$ and $O_{3 \Rightarrow 4}$ in preparation for ligation (see lower part of figure). All oligonucleotides are written 5' to 3' except O_{3*}.

Expressing compositions of mixtures –

Tomislav Cvitaš

In much of science we are interested in the qualitative and quantitative composition of mixtures. Since the fields of application are wide ranging including solid state physics, astronomy, environmental sciences, medicine, agriculture, etc., different terminology and symbolism has developed. Here we describe a classification of physical quantities used in expressing the composition of mixtures based on international recommendations[1–3] and standards[4,5] and relate them to the current practice.

A mixture consists of two or more pure substances. A solution is a special case, when one substance – the solvent – is treated differently from the others.[6]

The size of a sample can be described by any of the four extensive quantities: mass (m), volume (V), number of molecules or other entities building up the sample (N) or chemical amount (amount of substance, often called the number of moles, n). Which of these is chosen depends on convenience. Mass and volume have the advantage of being easier to measure, while number and chemical amount of entities are more amenable for theory, for mutual comparisons and understanding of chemical equilibria and kinetics.

Since the composition of a mixture does not depend on the size or extent of the sample, it is expressed by an intensive quantity. Such intensive quantities can be obtained by division of any of the above extensive quantities with another extensive quantity for the whole sample or for another substance in the mixture. There are several ways in which one can do this depending on convenience either of measurement or application. The derived quantities can be divided into four groups: *ratios*, *fractions*, *concentrations* and *molality*. In clinical chemistry a fifth group of quantities is used which are called *contents*.[3]

Ratios

For a mixture of two or more substances, it is often convenient to define the ratio between two substances. We shall denote the substances with indices i or j, but when it is necessary to denote the molecules, i.e. whenever amounts or numbers of molecules are used, we shall use the index A for the reference substance (usually the solvent) and B otherwise. (For example, while it is sufficient to say that the mass of sulfur in a sample is, m_S = 256 mg, when we talk about numbers and chemical amounts we have to specify the entities counted, and if the amount of S_8 molecules is 1 mmol the amount of atoms is n_S = 8 mmol. The subscript S has different meanings in the different cases.) Depending on which extensive physical quantity is used to express how much of a substance is present, we can define three types of ratios:

Name	Symbol	Definition
mass ratio	$\zeta_{i,j}$	$\zeta_{i,j} = m_i/m_j$
volume ratio	$\psi_{i,j}$	$\psi_{i,j} = V_i/V_j$
(chemical) amount ratio, mole ratio, number ratio	$r_{B,A}$	$r_{B,A} = n_B/n_A = N_B/N_A$

However, ratios are not commonly used. Neither IUPAC nor IUPAP explicitly recommend symbols for these quantities. ISO[4,i] recommends only the amount ratio (calling it the mole ratio). The other symbols listed were adopted from the German standard[5] which in addition recommends R for number ratio although it is identical with the amount ratio r. It is important when ratios are used to clearly state which substance of the mixture is chosen as the reference. In solutions, it is usually the solvent and the second index is often omitted, but in general it has to be clearly stated. Sometimes in the description of a preparation procedure it is said that two liquids are taken in their volume ratio. Mass and amount ratios are often used to describe the quantitative relationship between substances in reaction mixtures, but the symbols are hardly ever used.

Fractions

A fraction describes how much of the total property of the sample is contributed by one of the substances in it. As for ratios we can distinguish three types of fractions:

Name	Symbol	Definition
mass fraction	w	$w_i = m_i/\Sigma\, m_j$
volume fraction	φ	$\varphi_i = V_i/\Sigma\, V_j$
(chemical) amount fraction, mole fraction, number fraction	x, y	$x_B = n_B/\Sigma\, n_C = N_B/\Sigma\, N_C$

Since the number of entities is proportional to the chemical amount of entities and the proportionality constant is equal for all substances, $N_B = Ln_B$, where L is the Avogadro constant, the amount fraction is identical with the number fraction. The German standard,[5] however, lists the number fraction separately with the symbol X. The symbol x for amount fraction is used for condensed phases, while y may be used for gases.

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Fractions are frequently used to express how much of a substance is contained in a sample. They are all dimensionless quantities with values between 0 and 1 and the most common units used are the percentage,% (= 10^{-2}), and for lower values part per million, ppm (= 10^{-6}). It should be noted that the quantities in the denominator refer to values prior to mixing. This is important for volume fraction, since the sum of volumes of all the substances is not generally equal to the total volume of the mixture, and a confusion with volume concentration, see below, might occur.

Concentrations

Concentrations are physical quantities describing the ratio of one of the extensive quantities of a single substance (mass, volume, chemical amount or number of entities) to the total volume of the mixture, V. Thus there are four kinds of concentrations:

Name	Symbol	Definition	SI unit	Common units
mass conc.	γ, ρ	$\gamma_i = m_i/V$	kg m^{-3}	g/L = g dm^{-3}
volume conc.	σ	$\sigma_i = V_i/V$	1	1
amount conc.	c	$c_B = n_B/V$	mol m^{-3}	mol/L = mol dm^{-3}
number conc.	C	$C_B = N_B/V$	m^{-3}	cm^{-3}

All concentrations have different dimensions and different units. Mass concentration is a practical quantity used for preparing solutions, because both the mass of the solute and the volume of the solution can be measured. The common units are g/L, g/100 mL, etc. Volume concentration is rarely used (only the German standard[5] recommends it) and care has to be taken not to confuse it with volume fraction. When the sum of volumes of all substances is equal to the total volume of the mixture, the two quantities become identical. When using volume concentrations this has to be clarified. The chemical amount concentration (amount of substance concentration, previously called molarity) is the most frequently used quantity for expressing the composition of solutions since it enables a quick and chemically meaningful comparison of different solutions, and measured rates and equilibria are directly related to amount concentration. When there is no ambiguity, the amount concentration may be abbreviated to the single word 'concentration'. The previously used term molarity for amount concentration and the corresponding symbol M for mol/L are no longer recommended, although still widely used. The most common units for amount concentration are mol/L (= mol dm^{-3}) and its submultiples mmol/L, μmol/L, etc. The number concentration is usually used in describing gaseous mixtures and the common unit is cm^{-3}.

Molality

The molality is defined as the chemical amount of a solute divided by the mass of the solvent. Its recommended symbol is m, or alternatively b, to avoid confusion with mass, as we shall do here.

$$b_B = n_B/m_{solv}$$

Indeed, the German standard[5] recommends only b as symbol for molality and the new International standard ISO 31-8[4,1] lists b before m. Molality is often used in thermodynamic treatments and has the advantage over amount concentration in being temperature independent. The common unit is mol/kg.

Contents

Contents are quantities describing the ratio of one of the extensive quantities of a substance in the mixture (mass, volume, chemical amount or number of entities) to the total mass of the mixture,m. Since the sum of masses of all substances in the mixture is equal to its total mass, mass content is identical with mass fraction and is therefore redundant. Thus there remain only three contents:

Name	Symbol	Definition	SI unit
volume content	κ	$\kappa_i = V_i/m$	m^3 kg^{-1}
amount content	k	$k_B = n_B/m$	mol kg^{-1}
number content	K	$K_B = N_B/m$	kg^{-1}

Contents are rarely used in chemistry and not listed in the major documents on quantities and units.[1,2,4] Two such contents (number content and amount of substance content) are mentioned in clinical chemistry,[3] but no symbols are recommended.

Example

By mixing 70 mL of ethanol and 30 mL of water at 20 °C one obtains 96.8 mL of solution. The densities of ethanol and water at 20 °C are 0.7893 and 0.9982 g cm^{-3}, respectively, so that one can calculate all the quantities describing the composition of this mixture:

Ratios	
volume ratio	ψ(EtOH,H_2O) = 7: 3
mass ratio	ζ(EtOH,H_2O) = 1.84: 1 ~ 11: 6
amount ratio	r(EtOH,H_2O) = 0.721: 1 ~ 3: 4
Fractions	
volume fraction	φ(EtOH) = 70%
mass fraction	w(EtOH) = 64.8%
amount fraction	x(EtOH) = 41.9%
Concentrations	
mass concentration	γ(EtOH) = 57.1 g/L
volume concentration	σ(EtOH) = 0.723
amount concentration	c(EtOH) = 12.4 mol/L
number concentration	C(EtOH) = 7.47 × 10^{21} cm^{-3}
Molality	
molality	b(EtOH) = 40 mol kg^{-1}
Contents	
volume content	κ(EtOH) = 822 mL kg^{-1}
amount content	k(EtOH) = 14.1 mol kg^{-1}
number content	K(EtOH) = 8.49 × 10^{21} g^{-1}

Note, that when a volume change occurs during mixing the volume concentrations of all the substances in the mixture do not add up to unity.

Common practice

Some of the most frequent deviations from recommended usage are commented below.

The term concentration is often used as a general term for any of the quantities listed here. Thus, fractions are often called concentrations and one can deduce that fractions are implied only from the units. Furthermore, since all fractions are dimensionless, a decoration is frequently added to the symbol of the unit in order to specify which fraction is meant. Such practice is not recommended as symbols of units should never be changed to describe the quantity being measured. Instead of saying 'the concentration is one ppmv', we should say 'the volume fraction is 1 ppm'; instead of 'concentration of 12%w/w' one should say 'mass fraction of 12%', etc. In dilute aqueous solutions, mass concentrations expressed in milligrams per litre are almost equal to mass fractions expressed in parts per million. Here again one finds expressions such as 'concentration of nickel equals 2.6 ppm' instead of 'mass concentration of nickel equals 2.6 mg dm^{-3}'.

In atmospheric chemistry, the term mixing ratio is often used to denote a volume fraction or number fraction. Even if the term applied to a ratio, e.g. with respect to standard dry air (which is never mentioned, but is nearest to what is meant), the attribute 'mixing' does not give additional information, but creates ambiguity – whether a mass, volume or number ratio is meant.[7] Authors again resort to prohibited decoration of unit symbols.

Since fractions are numbers, the units are also numbers and as opposed to other units of measurement, they are known exactly and not subject to measurement. The most frequently used unit is the percentage, % (= 10^{-2}). It is the only such unit accepted by ISO.[4] IUPAC[1] also recommends the unit part per million, ppm (= 10^{-6}), which is also used in CODATA documents[8] and as 'part in 10^6' in the IUPAP document[2] for expressing relative uncertainties of precise measurements. However, one often encounters a much larger variety of units and symbols which necessarily leads to confusion. In continental Europe, a permille, ‰ (= 10^{-3}) is a common unit for expressing the mass fraction of alcohol in blood or for the salinity of sea water, while in some other parts of the world parts per thousand (ppt) are used. For very low values, units based on the American system of counting such as parts per billion, ppb (= 10^{-9}), parts per trillion, ppt (= 10^{-12}), etc. are often used. However, in Europe a billion is $(10^6)^2 = 10^{12}$, a trillion $(10^6)^3 = 10^{18}$, etc. No international recommendation of such units can therefore be agreed upon, and a different system based on SI prefixes would be welcome. The present status, and some possible solutions, for future recommendations are summarized in the Table.

	Symbol (present)		Version (to consider for future)		
Value	practice	recommended	1	2	3
10^{-2}	%	%	%	%	%
10^{-3}	‰,ppt		‰	‰	ml
10^{-6}	ppm	(ppm)	ppM	ppm	μl
10^{-9}	ppb		ppG	ppg	nl
10^{-12}	ppt		ppT	ppt	pl
10^{-15}	ppq		ppP	ppp	fl

The ideal situation, where practice and recommendation are in agreement, can be found only with the use of percents. The symbol ppm in parentheses denotes that ISO does not recommend its use. The three proposed future versions are based on SI prefixes. Version 1 is based on prefixes for multiples (mega, giga, tera and peta) with an unusual use of the prefix to be standing on its own (e.g. part per mega) and in the symbol being at the end. Version two uses the same system with lower case letters, but with the advantage of agreeing with current practice in two instances. Version three makes proper use of the symbols for prefixes, but introduces a new symbol l (or Roman one) for one.

Conclusion

The term concentration has two recommended meanings: (i) the name for a group of four quantities referring to the total volume of a mixture and (ii) the short form for amount (of substance) concentration. The use with a third, more general meaning found in the literature for any quantity describing the composition of a mixture should be discontinued as it leads to confusion. The adherence to recommendations by international organizations and scientific unions on the use of quantities and units should bring coherence and avoid misunderstandings in communication between scientists. An effort should therefore be made by all scientists and especially those involved in interdisciplinary research to become familiar with the recommendations and to follow them whenever possible. On the other hand the international commissions should seek solutions for confusing issues, consult as many scientists as possible, and finally produce recommendations acceptable to all involved.

I am grateful to Professors Ian Mills (University of Reading, UK) and Robert Alberty (MIT, Cambridge, MA) for reading the manuscript and making many helpful suggestions.

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(d) ISO 31-3:1992 Quantities and Units – Mechanics
(e) ISO 31-4:1992 Quantities and Units – Heat
(f) ISO 31-5:1992 Quantities and Units – Electricity and Magnetism
(g) ISO 31-6:1992 Quantities and Units – Light and Related Electromagnetic Radiations
(h) ISO 31-7:1992 Quantities and Units – Acoustics
(i) ISO 31-8:1992 Quantities and Units – Physical Chemistry and Molecular Physics
(j) ISO 31-9:1992 Quantities and Units – Atomic and Nuclear Physics
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(*n*) ISO 31-12:1992 Quantities and Units – Characteristic Numbers
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The role of chemistry in materials science and engineering

J. Economy

What is materials science and engineering?

Today, there are at least 100 departments in universities in the USA that are referred to as Materials Science and Engineering (MSE). For the most part they had their roots in pre-existing metallurgy and ceramics programs. Today, the field of MSE can include a number of other disciplines as indicated in Table 1. The interesting feature of Table 1 is the potential to describe this field as a matrix with considerable overlap in subject matter. This makes it possible to provide students with a much broader base of knowledge when compared with approaches which focus either on metals, ceramics or polymers. Another important feature of the field of MSE is illustrated in Fig. 1 which effectively describes the skills which students are expected to master before graduation. Students educated in this manner are thus equipped to enter industry with a Bachelor degree and contribute almost immediately to the needs of their employers.

One might ask what is the role of chemistry in the field of MSE? Chemistry as well as physics are critical building blocks for a successful career in MSE. In particular, synthesis of materials is a skill unique to chemistry and provides the knowledge-base essential to design new materials. Similarly, a knowledge of physical, inorganic, organic and analytical chemistry is highly desirable in addressing the many technical questions that arise in the development and understanding of new materials.

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Table 1. Matrix describing interdependencies between various materials disciplines

	Composites	Electronic materials	Biomaterials
Ceramics	A	A	B
Metals	A	A	B
Polymers	A	A	A

A = a critical interdependancy.
B = some areas of overlap.

The current increasing emphasis by industry and funding agencies on relevance and manufacturability is leading to further modifications of MSE curricula to include greater emphasis on design courses and activities that bring the student into direct contact with industry at a much earlier stage of their undergraduate program.

Examples of materials R&D which depend on a knowledge of chemistry

- Cross-linked Aromatic Copolyesters;
- Boron Nitride Matrix for Advanced Composites;
- Carbonaceous Materials for Environmental Control.

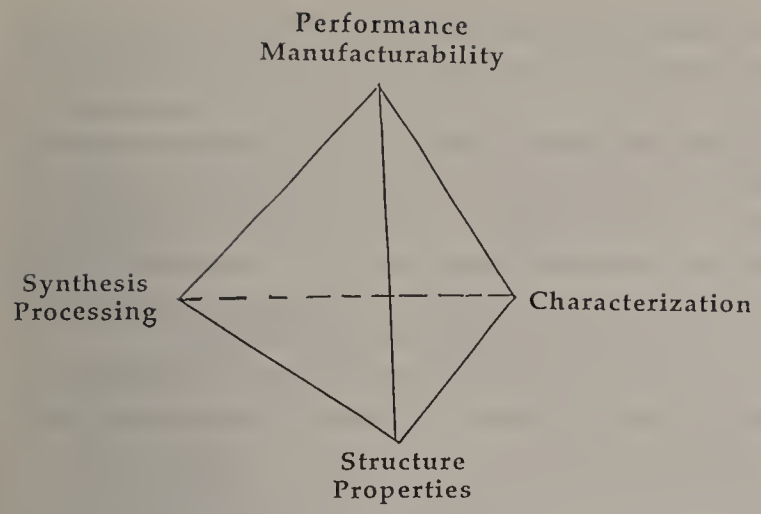

Figure 1. Areas of emphasis in an MSE curriculum.

Where appropriate, I will indicate the origins of these studies as well as their possible relevance to societal needs.

Cross-linked aromatic copolyesters

This study grew out of early work on the commercialization of liquid crystalline polyesters (LCP), and, to a lesser extent, a flame resistant fibre derived from a cross-linked phenolic resin. This work was made possible by use of new synthetic techniques. In the ensuing years, commercial development of LCPs has been adequate, but has not fulfilled early expectations.[1,2] As a result of shortcomings such as high cost and poor interlaminar shear properties, we undertook to prepare a cross-linked version of these aromatic copolyesters. We felt that the possibility for rapid interchain transesterification reactions at elevated temperatures would provide the potential for bonding of the cross-linked copolyester (see Fig. 2) providing a new degree of freedom in processing of these thermosetting resins.[3] It was relatively easy to design easily processible oligomers which would melt and wet surfaces such as fibre lay-ups. Subsequent curling and consolidation could be achieved in a relatively straight-forward fashion as indicated in Fig. 2.

One other feature that is of increasing concern to the field of thermosets is the requirements for recycling such materials. The cross-linked aromatic copolyester appears to be unique in this respect since we have found that we can depolymerize the cross-linked structure with acetic acid by heating at elevated temperatures. This process can be controlled so as to obtain an oligomer which can be re-cured into the same kind of thermoset resin.

This new family of cross-linkable copolyesters displays a number of other important advantages and these are summarized in Table 2. As a point of comparison, thermosets such as phenolics and epoxies begin to degrade on heating in air at 150 °C, absorb moisture from 1.5–6% and are not recyclable.

Finally, the role of synthesis can be illustrated rather dramatically by enumerating a number of new end uses that have developed based on the knowledge generated from this research. Thus, greatly improved dielectric insulators, structural foams, and adhesives have been prepared, while new types of lubricants and thermoplastic elastomers have been synthesized. In fact, some improvements may now be possible in the design of lower cost, higher performance LCPs.

Boron nitride matrices for advanced composites

In the mid 1960s a new type of composite was commercialized consisting of carbon fibres in a carbon matrix (C/C). This system displayed outstanding thermomechanical properties and could survive temperature cycles of at least 1000 °C and even to 2000 °C. Because of these features, these composites found immediate application as brakes for high speed aircraft. Over the ensuing years this market has grown rapidly so that today it appears to be approaching a billion dollar industry. On the other hand, the C/C system has a number of shortcomings including: (1) a costly manufacturing process involving repeated resin impregnations and charring followed by a chemical vapour infiltration of carbon and (2) potential for oxidative degradation during temperature excursions over 425 °C.

Several years ago we undertook a program to see if we could come up with an alternative to the carbon matrix using boron nitride (BN). It is well known that carbon and BN are structurally very similar but differ in that graphite is an electrical conductor and BN is an insulator. In some earlier work in the 1960s we had prepared BN fibres and identified some key advantages over carbon fibres including greatly improved oxidation resistance. We also showed in some recent work that we could prepare a C/C composite in one step by using as the matrix precursor an aromatic diacetylene oligomer. This oligomer gave a 95% carbon yield on heating to 800 °C, which allowed us to complete the process of carbonization in less than an hour. At about that time we learned that borazine would form an

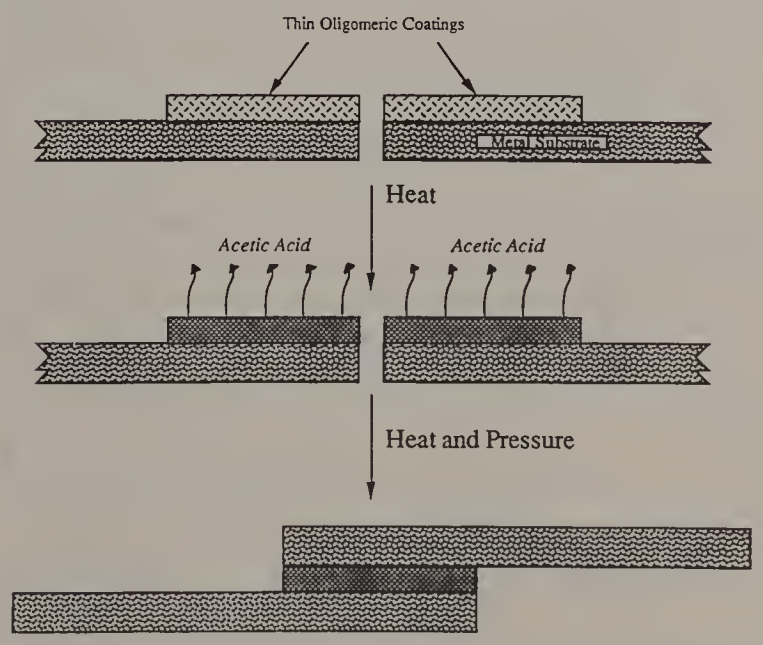

Figure 2. Process of solid state adhesion of cross-linked copolyesters.

Table 2. Key features of the new cross-linked aromatic copolyesters.

• Retention of properties	200 °C	(100%)
	350 °C	(60%)
• Low moisture pick-up		0.1%
• Potential for recycling		
• Relatively low-cost starting materials		
• Readily processed as		
- matrices for composites		
- adhesives		
- structural foams		
• Oligomers can display liquid crystalline character		

oligomer on heating at modest temperatures. Further heating of the oligomer to 1200 °C produced an unstable version of BN with an interlayer spacing of 3.56 Å (stable BN has a value of < 3.36 Å). We were able to show that the borazine oligomers could be designed to easily impregnate a carbon fibre lay-up and that with a suitable heating cycle one could obtain a very stable BN matrix in a yield of 90%.[4] As shown in Fig. 3, the process for fabricating these composites could be completed in 3–4 days as compared to several months typically required for the manufacture of C/C composites. Also, very high composite densities could be achieved using vacuum infiltration techniques.

Of considerable surprise to us was the unusually high mechanical properties of C/BN composites since one would predict a major problem due to a mismatch in coefficient of thermal expansion (CTE) between the anisotropic fibre and isotropic matrix. We suspected that the oligomeric borazine might display liquid crystalline character which would lead to sufficient orientation at the fibre surface to reduce the stresses associated with a CTE mismatch. In fact, mass spectrographic analysis indicated presence of a condensed polynuclear borazine structure, a necessary requirement for forming a discotic liquid crystalline phase.

It should be apparent from the above discussions that, to date, synthesis and characterization have been key ingredients to the success of this program. We are now launched on a program to develop low cost synthetic route to borazine which currently can only be purchased for $10 000/lb. We have already come up with a route which yields borazine for $250/lb and are exploring completely new approaches to bring the cost down to $10/lb.

Carbonaceous materials for environmental control

High surface area carbon in the form of charcoal and granules have been used routinely for many years to trap contaminants from air and water. In spite of the seeming importance of this field very little work has been carried out to develop new or improved carbonaceous systems or even more essential, to generate a basic understanding of how these materials function. Presumably, with such knowledge one could design carbon-

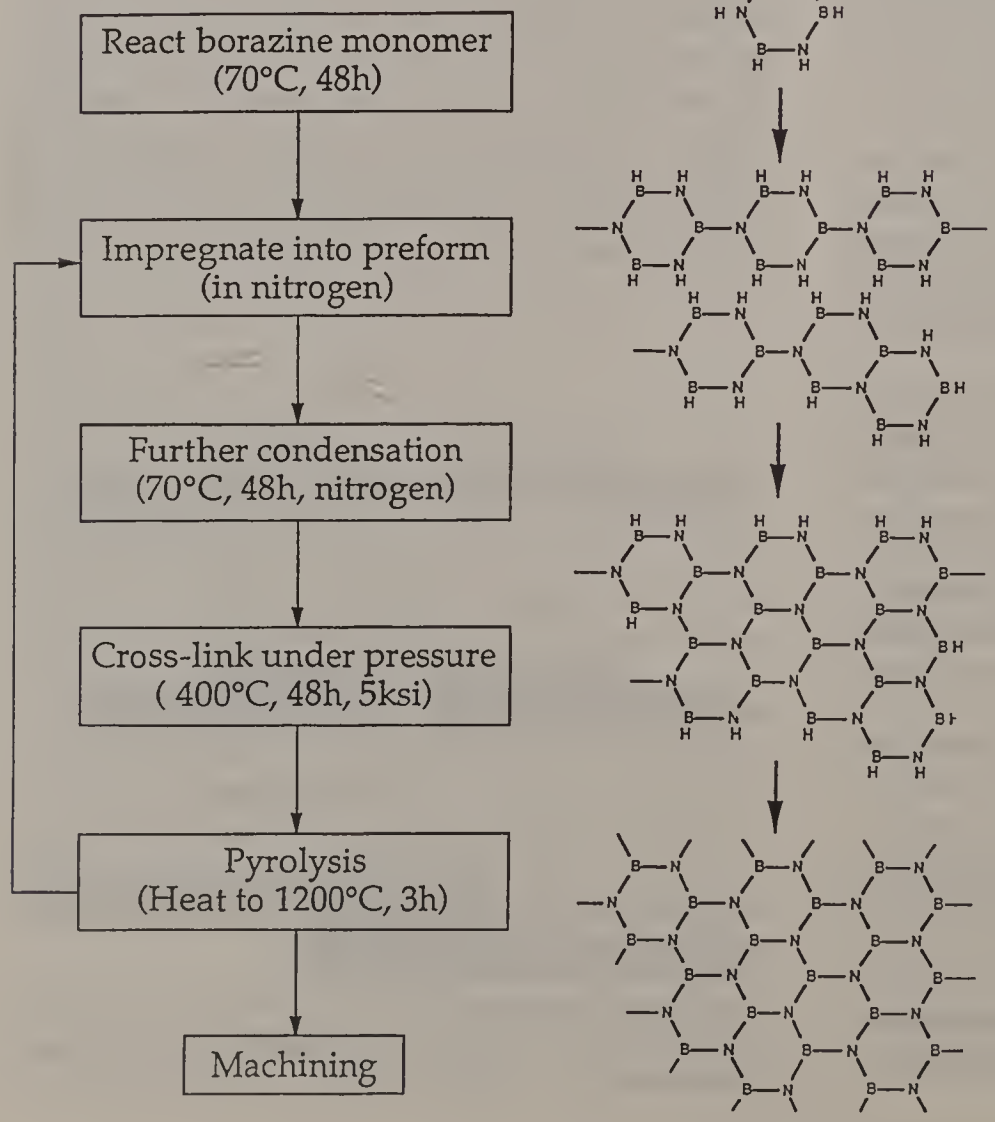

Figure 3. Flowchart for fabrication of C/BN composites.

Table 3. Areas of need for improved environmental control systems.

• Groundwater contaminants	industrial/nuclear/military
• Global air contaminants	freons/SO_x/CO_2
• Work-place environment	solvents
• Quality of air in home	pollen/CH_2O/radon
• Improved industrial processes	recovery & recyclability
• Toxic warfare	gases/bacteria/viruses

aceous systems tailored to remove contaminants at the level of a few parts per billion (ppb) without the excessive cost penalties usually ascribed to removal of contaminants at even a few parts per million (ppm).

About 1970, we developed and commercialized a high surface area carbon fibre which appeared to offer important advantages over activated carbon granules. These included much higher adsorption capacity, improved contact efficiency, and greatly simplified techniques for regeneration. This product has proven to be very successful commercially even though its cost may by 100-fold that of the granules or powders.

More recently, we undertook a program to develop a much better understanding of the mechanism of adsorption of various contaminants, and also to design new, much lower cost, carbonaceous fibre systems. Initially, our work focused on determining what the chemical nature of the micropore surface was and could we control it. At the same time we wanted to better understand the nature and role of the micropore dimensions. Such a basic understanding is essential if one is to develop solutions to the many environmental problems facing the developed countries of the world. See

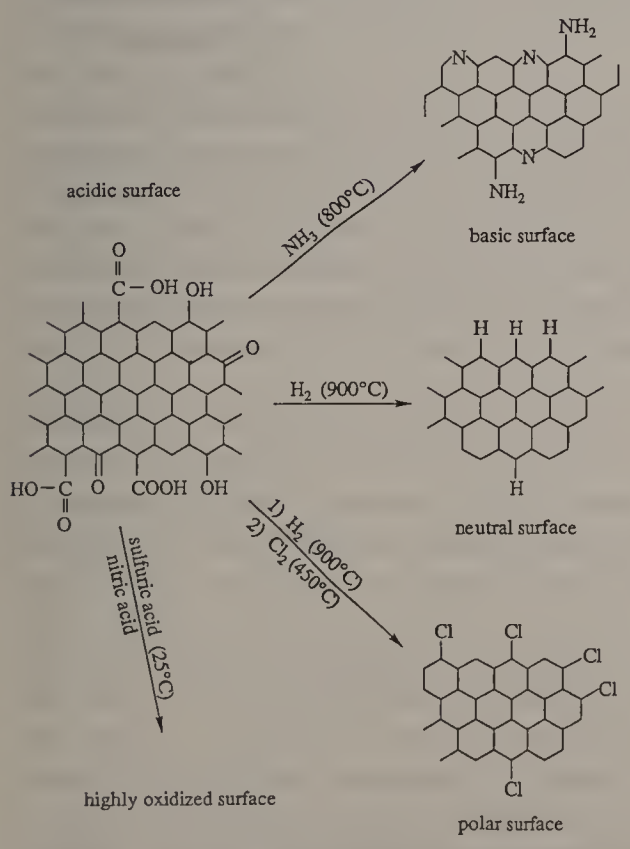

Figure 4. Chemical reactions on activated carbon fibres.

Table 3 for a listing of some of these problems.

As one might expect, the nature of the carbon micropore surface is determined by the, etchant used to create the pores. Since the etching environment is usually oxidizing one will generate phenolic hydroxyls, guinones and possibly carboxylic acids at the pore surface at oxygen concentrations of several percentage. What we have found is that pore surface chemistry can be altered as indicated in Fig. 4 to produce basic, neutral, polar and much more acidic surfaces. Extensive evaluation of such surfaces using a wide range of contaminants shows a direct correlation between the adsorption capacity and the nature of the surface.

We have also found that the pore size and shape play a critical role in determining the adsorption capacity at low concentrations. Thus the higher surface area carbon displays a much higher capacity at high contaminant concentrations, while at low concentrations the low surface area system is far more efficient. This cross-over in capacity is directly related the overlap potentials within a pore which are essential for adsorbing contaminants at low ppm or even ppb It should be apparent that as one optimizes both the pore size and shape and the pore surface chemistry the potential exists for developing highly selective adsorption systems. We have also been able, for the first time, to image the pore surface using scanning tunnelling microscopy and to establish an excellent correlation between pore size and shape vs. surface area.

With these new insights, we are now developing new kinds of low cost adsorption and separation systems and are currently working with several companies to evaluate some of these new systems. The significance of this work is perhaps best demonstrated from a brief perusal of the many environmental problems facing society today (See Table 3).

It should be apparent from the above that there is a strong interdependency between the fields of MSE and chemistry. To generalize, most of the important innovations in design of new materials have their origins in a knowledge of chemical synthesis. At the same time, such innovations are only possible from a detailed understanding of structure property relationships and their dependency on synthesis and processing.

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38th IUPAC Council Meeting

Elections of Officers and Bureau members

According to Statute 5.401, the 38th IUPAC Council must elect:

- Officers of the Union;
- Elected Members of the Bureau.

Nominations for the various positions that fall vacant at the end of 1995 were required by the Secretary General at the IUPAC Secretariat before 10 June 1995, i.e. 2 months before the start of the Council meeting (Bylaw 2.221). The following are details of vacancies and candidates who had been nominated by the time this issue went to press (25 April 1995).

Officers

President

Prof. A. E. Fischli (Switzerland), Vice-President and President-Elect, becomes President on 1 January 1996 (Statute 4.2).

Vice-President – Vacancy

The Vice-President to be elected at the 38th Council will be President-Elect, and will become President on 1 January 1998.

Prof. Joshua Jortner has been nominated for the position of Vice-President.

Prof. Joshua Jortner is President of the Israel Academy of Sciences and Humanities, he is a physical chemist of international renown, well known for his work on intramolecular and condensed phase dynamics. He has been the recipient of many international prizes, including the Wolf prize in chemistry (1988). He is a member of the Executive Committee and the Bureau of IUPAC and of the Subcommittee on Ethics in Science.

Past-President

The retiring President, *Prof. K. I. Zamaraev* (Russia), will remain an Officer (Statute 6.1) and a member of the Bureau for a period of two years (Statute 7.2).

Secretary General – Vacancy

Prof. G. den Boef (Netherlands), the present Secretary General, completes his period (August 1991 – December 1995) of service, and has decided not to seek a second term (Statute 6.52).

Nominations for Secretary General

Dr Edwin D. Becker (USA)

Dr Edwin D. Becker was born in 1930 and received his BS, in chemistry, from the University of Rochester, Rochester, NY, in 1952 and his PhD from the University of California at Berkeley in 1955.

Dr Becker has spent the major part of his career at the National Institutes of Health near Washington, DC. He has been: Chief of the Molecular Biophysics Section, 1961–72; Chief of the Laboratory of Chemical Physics, 1972–80; Associate Director for International Research, 1979–81; Associate Director for Research Services, 1980–88; Chief of the Laboratory of Analytical Chemistry, 1988–present. Dr Becker has, since 1959, been a Professorial Lecturer at the Georgetown University, Washington, DC, where he teaches graduate-level courses.

Dr Becker is internationally known for his research in molecular spectroscopy, and nuclear magnetic resonance (NMR), and for his two books on NMR. He has published about 100 papers in vibrational spectroscopy and hydrogen bonding. He has extensive administrative experience at the National Institutes of Health, where for eight years he managed research services with about 1300 employees and an annual budget in excess of $150 million.

IUPAC Activities: Ted Becker has been active in IUPAC during the last 22 years, including service as Chairman of the Commission on Molecular Structure and Spectroscopy, 1975–81; Secretary of the Physical Chemistry Division, 1981–85; Chairman of the Commission on Publications, 1987–94; and Chairman of the United States National Committee for IUPAC, 1984–86. He has served on a number of other committees and boards and is currently the Chairman of the Committee on International Activities of the American Chemical Society.

Awards: Include, Coblentz Prize, 1966, in Vibrational Spectroscopy; Fellow of the American Association for the Advancement of Science, 1988; Bicentennial Medal, Georgetown University, 1989, and Foreign Fellow of the National Academy of Sciences, India, 1992.

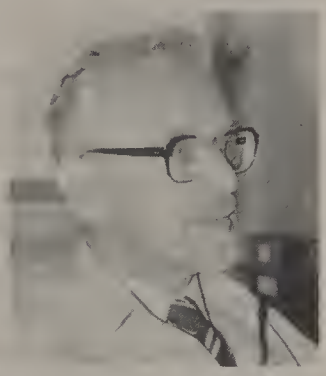
Other positions: American Chemical Society, Committee on International Activities, 1987–present, Chairman, 1993–present; Joint Committee on Atomic and Molecular Physical Data, 1967–89, Chairman, 1978–81; Federal Executive and Professional Association Board, 1973–83, President, 1982–83; Editorial Board, *Journal of magnetic Resonance*, 1969–present, and Section Editor, *Encyclopedia of Nuclear Magnetic Resonance*, 1992–present.

Treasurer – Vacancy

Prof. J. M. Ward (UK), the present Treasurer, is eligible for re-election, having completed four years (January 1992 – December 1995) of service (Statute 6.52). Prof. Ward has been renominated.

Nominations for Treasurer

Prof. John M. Ward (UK)



John Mason Ward is married with a daughter and two sons, and has four grandchildren. He started his professional career in paper manufacturing, this was, however, interrupted by the Second World War during which he worked on chemical defence at Porton Down. At the end of hostilities, he joined the Electricity Supply Industry to work on washing processes to remove sulfur from flue gases.

In 1949, he was appointed to a group of 12 chemists and engineers at the Central Electricity Research Laboratories, Leatherhead, to build up a chemistry research team. When he retired as Research Manager and Head of the Chemistry Division, the total strength of the Laboratory was 800 with 80 in the Chemistry Division. Prof. Ward was earlier responsible for building up a Materials group and a Biology group which later became independent divisions.

The principal subjects of research by the Chemistry Division were atmospheric pollution, removal of sulfur from flue gases, analytical methods and instruments for monitoring micro quantities of impurities in boiled feed water, and corrosion at high temperatures and high pressures in conventional and nuclear power stations. He and his team were awarded the Royal Society Esso Gold Medal in 1977 for their work on corrosion prevention.

In 1969, he was appointed Visiting Professor in the Chemistry Department of the University of Surrey, an appointment he still holds in an honorary capacity.

Since 1964, he has held various offices in the Royal Institute of Chemistry and the Royal Society of Chemistry. Amongst those were: Vice-President (Royal Institute of Chemistry) 1970–72, Treasurer (Royal Institute of Chemistry) 1976–80, Treasurer (Royal Society of Chemistry) 1980–86, President (Royal Society of Chemistry) 1988–90.

He joined the IUPAC Finance Committee in 1986 and succeeded as Chairman in 1990. He was elected Treasurer of the Union for 1992–95.

Bureau – four Vacancies (minimum)

According to Statute 7.2 the Bureau consists of the Officers, the Presidents of the Divisions/Sections, together with not less than 10 other members elected by Council, who shall be known as 'Elected Members'. At the conclusion of the 37th Council in Lisbon, there were 10 Elected Members of the Bureau. At the 38th Council the Bureau will make recommendations to Council as to the number of Elected Members (10 or more), who should be on the Bureau for the succeeding two years.

Elected Members are elected for a period of four years, and they are eligible for election for a second period of four years.

No Adhering Organization shall have more than *one Elected Member* of the Bureau. Stature 7.2 also states that 'the principle of fair geographical representation of Members shall be taken into account'.

Elected Members of Bureau, retiring in 1995, who are not eligible for re-election, but may be nominated for another office:
Prof. M. T. Beck (Hungary);
Prof. G. Modena (Italy);
Prof. J. Jortner (Israel);

Elected Member of Bureau, retiring in 1995, but who is eligible for re-election for a further 4-year period:
Prof. A. Chakravorty (India);

Elected Members of Bureau, who were elected at the 37th Council until 1997:
Prof. R. D. Brown (Australia);
Dr D. F. Eaton (USA);
Prof. E. J. Grzywa (Poland);
Prof. J. W. Lorimer (Canada);
Prof. L. K. Sydnes (Norway);
Prof. C. Zhang (Chinese Chemical Society).

At least four Elected Members of the Bureau must be elected at the 38th Council in Guildford, i.e. the minimum number of 10 Elected Members (Statute 7.2) less the six Elected Members who continue in office until 1997.

Nominations for Bureau

Prof. Animesh Chakravorty (India)

Prof. Chakravorty was born on 30 June 1935, and is married with two children.

Education and Career: He gained his PhD from Calcutta University in 1961 and was subsequently: Lecturer, Vidyasagar College 1959–62; Research Associate at MIT and Harvard University 1961–64; Lecturer, Assistant Professor, Professor, Head of the Department of Chemistry, Indian Institute of Technology Kanpur 1964–77; Professor and Head of Department, Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, India.

Scientific Organizations: At various times: Member and Chairman at Chemistry Sectional Committees of Indian National Science Academy and Indian Academy of Sciences; Member of Councils of both the aforementioned Academies; Council Member, Indian Chemical Society; Council Member, Indian Association for the Cultivation of Science; Member, Indian Science Congress; Member, Science and Engineering Research

Council and Chairman, Program Advisory Committee for Inorganic Chemistry, Department of Science and Technology; Member, Chemistry Committees of University Grants Commission and the Council of Scientific and Industrial Research.

At various times: co-ordinator, Indo-Russian Project on Structural Inorganic Chemistry and Organometallic Chemistry; Member, International Advisory Board, Eurasia Conferences; Visiting Professor Texas A&M University. Special Lecturer at many universities and institutes overseas; MIT-Harvard Inorganic Chemistry Colloquium, MIT; Gordon Research Conference, New Hampshire; International Conference on Co-ordination Chemistry, Colorado, Eurasia Conference on Chemistry, Bangkok; 75th Anniversary of Royal Australian Society, Melbourne; Bureau Member, IUPAC 1991 – today.

Awards and Fellowships: Shanti Swarup Bhatnagar Prize in Chemistry; Chemistry Prize of the Third World Academy of Sciences; T. R. Seshadri Commemoration Medal; Fellow, Indian National Science Academy; Fellow, Indian Academy of Sciences; Ajit Memorial Lecture Award; Baba Kartar Singh Lecture Award; National Lecture Award; Platinum Jubilee Lecture Award; Honorary Professor, Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore; Nehru Chair, University of Hyderabad.

Editorial Work: At various times: Journal of the Chemical Society Dalton Transactions; Inorganica Chemica Acta; Indian Journal of Chemistry; Proceedings of Indian Academy of Sciences; Proceedings of Indian Science Academy; Chemistry Education.

Research Activities and Interests: Inorganic chemistry, organometallic chemistry and bioinorganic chemistry; synthesis, structure and redox reactions of model systems. Published two hundred and 50 publications; trained nearly 50 PhD students, and numerous postdoctoral and other fellows.

Prof. Hitoshi Ohtaki (Japan)

Prof. Ohtaki was born 16 September 1932 in Tokyo and graduated from the Faculty of Science, Nagoya University. After Graduate School, Nagoya University, he was appointed Research Associate, Tokyo Institute of Technology, Lecturer and then Associate Professor, Nagoya University, Associate Professor and then Professor, Tokyo Institute of Technology, Professor of the Institute for Molecular Science and Director (Coordination Chemistry Laboratories), Institute for Molecular Science and also Professor and Dean of the Graduate University for Advanced Studies.

He was named Emeritus Professor of the Tokyo Institute of Technology and the Graduate University of Advanced Studies in 1993. He is at present, Professor of the Ritumeikan University and Director of the Institute of Science and Engineering. He is a member of the Science Council of Japan.

Prof. Ohtaki was a member of the Commission on Equilibrium Data of the Analytical Chemistry Division of IUPAC from 1975 to 1993 (Associate Member 1975–79, Titular Member 1979–85, Secretary 1981–83, Chairman 1983–85, National Representative 1985–89 and Coopted Member of the Division 1989–93). He was also a Division Member of Inorganic Chemistry from 1987 to 1991.

Prof. Ohtaki was the former President of the Japanese Society of Coordination Chemistry and is the current president of the Association of Japanese Solution Chemists. He is the Chairman of the Committee for International Affairs of the Chemical Society of Japan. He was the Chairman of the 2nd and 4th Eurasia Conferences on Chemical Sciences held in Seoul, Korea (1992) and Kuala Lumpur, Malaysia (1994), and the 30th International Conference on Coordination Chemistry, Kyoto, Japan (1994). He is the representative of the Chemical Society of Japan for the Federation of Asian Chemical Societies and the Vice-Chairman of the 1995 International Chemical Congress of Pacific Basin Societies (PACIFICHEM'95).

Research Activities and Interests: Solution chemistry and coordination chemistry.

Prof. Norman Greenwood (UK)

Education and Career: Norman Greenwood was born in Melbourne, Australia, 19 January 1925, and studied at the University of Melbourne (MSc, 1948; DSc, 1966) and at Cambridge University (PhD, 1951; ScD, 1961). Prof. Greenwood was awarded the D de l'Univ. *honoris causa* of the University of Nancy, France, in 1977, elected a Fellow of the Royal Society in 1987 and Foreign Associate of the Académie des Sciences, France, in 1992. He has been particularly active in both teaching and research and is well known for his work on both national and international committees.

Prof. Greenwood retired in 1992 as Professor of Inorganic and Structural Chemistry at the University of Leeds and is now Emeritus Professor of Chemistry. He was Dean of the Faculty of Science at Leeds (1986–88) and has held visiting professorships in Australia, Canada, Denmark, Japan, The People's Republic of China and the United States.

Prof. Greenwood has made numerous contributions to solid state chemistry, and his book, *Ionic Crystals, Lattice Defects and Nonstoichiometry* (1968) had considerable impact, being translated into German, Japanese and Spanish. He was one of the first to apply the Mössbauer effect to chemical problems and coauthored a definitive monograph in 1971. More recently, he has made major contributions to the reaction chemistry and structures of the boron hydrides and has opened up the new field of polyhedral metalloborane cluster chemistry. In all, he has published some 450

research papers and 10 books, the most recent of which, *Chemistry of the Elements*, broke new ground and has already been translated into German, Italian and Czech. Prof. Greenwood has received many national and international honours and awards. He has been: President of the Dalton Division of the Royal Society of Chemistry; President of the British Association for the Advancement of Science, Section B (Chemistry), and is at present Chairman of the Royal Society's Panel on Exchange Programs with Central and Eastern Europe.

IUPAC Activities: Norman Greenwood has been active in IUPAC affairs for many years, particularly as Chairman of the Commission on Atomic Weights (1969–75) and President of the Inorganic Chemistry Division (1977–81). More recently, he was with Prof. Yves Jeannin one of the two IUPAC members of the joint IUPAC-IUPAP Working Group on Criteria for the Discovery of the Transfermium Elements. He is the current Chairman of the British National Committee for IUPAC and is strongly committed to the present moves to modernize and develop IUPAC structures so as to make the Union more effective in dealing with emerging needs in the coming years.

Prof. Pieter S. Steyn (Republic of South Africa)

Pieter Streicher Steyn was born, 5 January 1940, in Vryburg, Cape Province, Republic of South Africa. He is married with three children.

Education and Career: Prof. Steyn studied in the University of Stellenbosch, Stellenbosch; BSc, 1956; BSc (Hons), 1962; MSc (*cum laude*); 1963, and then at the University of South Africa; PhD, 1966. Following a Postdoctoral Fellowship (1967–68) in the School of Pharmacy of the University of Wisconsin, Madison, USA, he was appointed to the National Chemical Research Laboratory, CSIR (1968–86) where he became Head of the Division of Organic Chemistry. From 1986 to 1987 he was Chief Director of the National Food Research Institute, CSIR, and from 1987 to 1992 he was Director of the Division of Food Science and Technology, CSIR. In December 1992, Prof. Steyn was appointed the first CSIR Fellow, this being the highest career position in science within CSIR. In October 1993, he was appointed Professor and Head of Department of Chemistry and SASOL Professor of Chemistry at the Potchefstroom University for Christian Higher Education, and Director of the SASOL Center of separation Technology.

Research Interests: Prof. Steyn's research career has been devoted to the isolation, analysis, structure elucidation, synthesis and biosynthesis of mycotoxins and, to some extent, other toxic and medicinally active substances from plants. This research has been undertaken with numerous groups within South Africa and with research groups in Australia, Europe and the United States. Prof. Steyn has authored or coauthored 150 scientific papers and 20 reviews.

Offices and Assignments: These include: Member of the Academy of Sciences of South Africa (1994–present); Vice-President of the South African Joint Council of Scientific Societies (1985–86); President of the South African Joint Council of Scientific Societies (1986–87); Member of the South African National Committee for IUPAC (1973–present); Vice-President of the Applied Chemistry Division of IUPAC (1989–91); President of the Applied Chemistry Division of IUPAC (1991–95); and President of the International Association for Cereal Science and Technology, Vienna (1992–94).

Since 1967, Prof. Steyn has given lectures at the Conventions of the South African Chemical Institute, at the Specialist Conference on Organic Chemistry, and been invited to speak at numerous international meetings.

Awards: Raikes Gold Medal of the South African Chemical Institute (1975), Gold Medal of the South African Chemical Institute (1987), CSIR Merit Prize (1987) – top award of the CSIR, Havenga Gold Medal for Chemistry (1992) from *Die SA Akademie vir Wetenskap en Kuns*, and Friedrich Schweitzer Medal (1993) from the International Association for Cereal Science and Technology, Vienna.

Dr Jean Rouquerol (France)

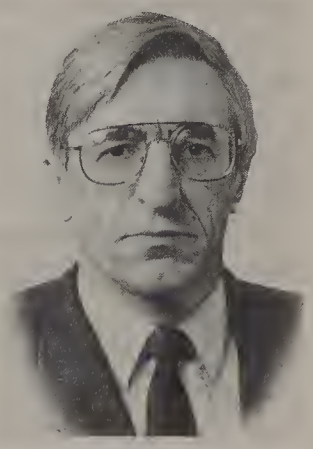
Jean Rouquerol was born in Paris on 1 October 1937; he is married with four children. He studied at the University of Paris (Sorbonne) where he received his Doctorat ès-Sciences Physiques, 1964, for work in the field of catalysis. Thereafter, he joined the staff of the Centre National de la Recherche Scientifique (CNRS) and was appointed in 1975, Deputy Director of the Centre de Thermodynamique et de Microcalorimétrie du CNRS, Marseilles, of which he has been Director since 1990.

His scientific interests deal mainly with powders and porous materials, with special attention to the kinetics and mechanism of their thermal preparation, transformation and adsorptive properties, either from a gas or a liquid, as studied from the thermodynamic viewpoint, i.e. state and phase changes undergone by the adsorbed layer. He is interested in the development of novel investigative tools for this research, mainly in microcalorimetry, thermal analysis and adsorption techniques. His main interest, due to its multiplicity of uses, is controlled transformation rate thermal analysis (CTRTA).

Dr Rouquerol is the senior author of about 110 research papers and reviews, and has given 90 oral presentations at conferences. He has been invited to present about 75 lectures, mostly out of France, he has coauthored four books and is a member of six editorial

boards of technical journals which publish research on interfaces (*Langmuir, J. Coll. Interface Sci.*) or with thermal analysis (*Thermochimica Acta*).

Offices and Assignments: Dr Rouquerol started his IUPAC activities as a member of the Subcommittee on Reporting Gas Adsorption Data (1976–84). He then entered the Commission on Thermodynamics (I.2) as an Associate Member (1981–85) and worked in a task group on the classification of calorimeters. Nevertheless, it is in the Commission on Colloid and Surface Chemistry Including Catalysis (I.6) that he has spent the majority of his time: Associate Member (1983–85), Titular Member (1985–93), Chairman of the Subcommittee for the Characterization of Porous Solids (1985–93) and then Chairman of the Commission (1991–93). He is deeply convinced of the capital role and possibilities of IUPAC in helping chemical scientists and engineers of any country to better understand each other and to efficiently address modern challenges.



Prof. O. M. Nefedov (Russia)
Oleg Matveyevich Nefedov was born in Dmitrov, Moscow Region, 25 November 1931. He is married with two children.

Education and Career: Prof. Nefedov graduated from the Institute of Chemical Engineering, Moscow, in 1954 and undertook graduate courses at the Mendeleev Institute of Chemical Technology, Moscow, between 1954 and 1957; in 1957 he was a Candidate of Sciences from the same institute and in 1967 became Doctor of Sciences (Organic Chemistry), Zelinsky Institute of Organic Chemistry, Moscow.

Between 1957 and 1968, Prof. Nefedov was a research scientist at the Zelinsky Institute of Organic Chemistry, Moscow; between 1959 and 1960 he held a Postdoctoral Fellowship in Heidelburg University, Germany, in the laboratory of Prof. Georg Wittig, and since 1971 he has been a Visiting Professor at Pennsylvania State University, USA.

In 1968, he was appointed: Head of Laboratory of Carbene and Small Ring Chemistry, Zelinsky Institute of Organic Chemistry, and Professor of Chemistry, Zelinsky Institute. In 1987, Prof. Nefedov was made a Full Member (Academician) of the USSR Academy of Sciences, subsequently, the Russian Academy of Sciences. He became Vice-President of the USSR Academy of Sciences, Russian Academy of Sciences, in 1988.

Prof. Nefedov is Editor-in-Chief of a number of journals, namely, Mendeleev Communications, Russian Chemical Bulletin (Izvestiya Akademii Nauk. Seriya Khimicheskaya) and the Russian Chemical reviews (Uspekhi khimii). He is currently the Supervisor of the National Scientific Technical Program 'Ecologically Safe and Resource-Savings Processes of Chemistry and Chemical Technology'.

Awards: USSR State Prize, Moscow, 1983 and 1990; Zelinsky Prize, Moscow, 1987; Prize of the USSR and Hungarian Academies of Sciences, Moscow, 1988; Semenov Prize, Moscow, 1991 and Karpinsky Prize, Hamburg, 1993.

Prof. Nefedov is an organic chemist with special interests in physical organic chemistry, small ring chemistry, organic synthesis and organometallic chemistry. He has authored numerous scientific papers and books.

Offices and Assignments: Titular Member of the Commission on Physical Organic Chemistry (III.2) 1981–91, and Associate Member of the Commission on Physical Organic Chemistry, 1991–93.

Prof. P. De Bièvre(Belgium)
Professor Paul De Bièvre was born in Blankenberge, Belgium, 7 July 1933, he is married with five children.

Education and Career: Prof. De Bièvre gained his Lic. Chemistry from the University of Ghent in 1955 and his PhD in 1959 also from the University of Ghent. From 1956 to 1961 he was an Assistant Lecturer at the University of Ghent, and in 1961 became a Lecturer in the University of Ghent. From 1961 to 1973, he was Section Head of Mass Spectrometry of Solids at the EC-Central Bureau for Nuclear Measurements (now called the Institute for Reference Materials and Measurements, IRMM), becoming Group Leader and Coordinator for Safety Programs in 1974. From 1972 to 1984, he was first: Lecturer in Inorganic Chemistry, and subsequently Lecturer in Inorganic Mass Spectrometry in the University of Antwerp. Becoming Professor of Isotope Mass Spectrometry and Stable Isotope Chemistry in the University of Antwerp in 1984.

His laboratory at IRMM provides the European Community, and other nations, with Isotopic Reference Materials, he is currently active in the three redeterminations of Avogadro's Constant which have been going on for the last 10 years; with PTB, Germany, IMG, Italy and NRLM, Japan.

Offices and Assignments: Include: IUPAC International Commission on Atomic Weights and Isotope Abundances: Observer (1971), Associate and then Titular Member (1973–85), National Representative (1985–present). Chairman of IUPAC Subcommittee on the Assessment of Isotopic Composition of the Elements, 1975–83. Chairman of the Working Group on Destructive Analysis European Safeguards Research and Development Association, 1975–present. Member of the Steering Committee of the USA Safeguards Analytical Laboratory Evaluation, 1978–81. Member, and subsequently President (1988–present) of the National Committee on Pure and Applied Chemistry of the Belgian Royal Academy. Member of the IUPAC Committee on Chemistry and Industry, 1987–present. Chairman of

the IUPAC LLTC Isotope-specific Measurements as References, 1987–93. Chairman of EURACHEM, 1993–present.

Prof. De Bièvre is President of the National Committee on Chemistry of the Belgian Royal Academy and has been an advisor to various IAEA programs and also to programs of the Belgian Nuclear Research Center in Mol, Belgium.

Awards: Stas-Spring award, Royal Academy of Belgium, 1960.

Prof. De Bièvre has been granted more than 20 patents in a number of countries. He has published about 90 scientific papers and has supervised 15 PhD students.

Prof. P. Kratochvíl (Czech Republic)

Professor Pavel Kratochvíl was born in Prague, February 1930.

Education and Career: In 1953, he became Master of Engineering, Institute of Chemical Technology, Prague, and until 1957 he was Lecturer on physicochemical principles of technological processes at the Institute of Chemical Technology, Pardubice. In 1957, he joined the Institute of Macromolecular Chemistry of the then Czechoslovak Academy of Sciences, where he is currently Director. Prof. Kratochvíl is also Professor of Macromolecular Chemistry at the Institute of Chemical Technology, Prague.

Prof. Kratochvíl is the author of 170 original communications in international journals, 10 reviews, one monograph and three contributions to monographs. His main field of research activity is the physical chemistry of polymers, particularly the investigation of solution properties of polymers and copolymers, and light scattering from polymer solutions.

Offices and Assignments: Within IUPAC, Prof. Kratochvíl started his activities as an observer in the Commission on Macromolecular Nomenclature in 1977. He became a Titular Member of this Commission in 1979 and served as its Chairman from 1985 to 1991. Since 1985, he has been a member of the Interdivisional Committee on Nomenclature and Symbols. He became a member of the Macromolecular Division Committee in 1994. He has been closely involved with various IUPAC-sponsored meetings which have been held in Prague, including the International Symposia on Macromolecules in 1965 and 1992, and most recently, of the Prague Meetings on Macromolecules (Microsymposia and Discussion Conferences).

Prof. Kratochvíl was the founding member of the Learned Society of the Czech Republic, he is a Fellow of the Royal Society of Chemistry, UK, and a member of numerous boards, both national and international. He is the holder of the Czechoslovak National Prize for Science, 1970, and the Prize of the Czechoslovak Academy of Sciences, 1977.

Prof. Dr Gerhard M. Schneider (Germany)

Professor Gerhard M. Schneider was born, 7 May 1932, in Neufechingen, Saarbrücken, Germany.

Education and Career: Prof. Schneider gained his *Abitur* in 1951 and was a chemistry student at the University of Saarbrücken, 1951–54, and, subsequently, at the University of Göttingen, 1954–57. He gained his *Diplomchemiker*, 1957, from the University of Göttingen, his *Dr rer. nat*. from Göttingen in 1959, and his *Habilitation* (Physical Chemistry) from the University of Karlsruhe in 1965.

Prof. Schneider was *Wissenschaftlicher Assistent*, 1958–61, at the University of Göttingen; *Wissenschaftlicher Rat*, 1965–69, and *Oberassistent*, 1961–65, at the University of Karlsruhe. Since 1969, he has been *Universitätprofessor* in the *Lehrstuhl für Physikalische Chemie* at the *Ruhr-Universität Bochum*.

Prof. Schneider's main field of research has been the thermodynamics of pure substances, and of mixtures, at high pressures. However, he has also investigated thermal methods of analysis (DTA and DSC) at high pressure, methods for separation (supercritical fluid extraction and chromatography) and the kinetics of phase separation by relaxation methods. His current interests include: phase equilibria of binary, ternary and quaternary mixtures with at least one supercritical component, and the spectroscopic study of such mixtures. He has published more than 250 papers in refereed journals and given more than 200 communications to scientific meetings.

Prizes: Nernst Prize of the *Deutsche Bunsengesellschaft für Physikalische Chemie*, 1969; Rossini Lecturer, Conference on Chemical Thermodynamics, Como, Italy, August 1990, and *Wilhelm-Jost Lecturer der Deutschen Bunsengesellschaft*, 1994–95.

Offices and Assignments: Within IUPAC, Prof. Schneider has been a Member, 1973–77; Secretary, 1977–81, and Chairman, 1981–85, of the Commission on Thermodynamics (I.2). He has also been a Member, 1981–85, and Secretary, 1985–87, of the Physical Chemistry Division Committee; and Vice-President, 1987–89, and President, 1989–91, of the Physical Chemistry Division.

Prof. Schneider has been a member of the Advisory Board of the Journal of Thermodynamics (Member, since 1975, and Chairman, 1980–90). He has also been a member of the Editorial Board of Fluid Phase Equilibria, 1977–90.

Prof. Okan Tarhan (Turkey)

Okan Tarhan was born, 18 March 1940, in Anatolia, Turkey, he is married with one daughter.

Education and Career: Prof. Tarhan gained his Dipl.Ing. in Chemical Engineering from the Faculty of Science of the University of Istanbul in 1963, an MSc in

Chemistry, 1966, and a PhD in Chemistry, 1968, from the University of East Anglia, UK.

He has been: Assistant Professor, 1969–73; Associate Professor, 1973–79; and Full Professor, 1979–present, at the Middle East Technical University, Ankara, Turkey. Also at the Middle East Technical University, Prof. Terhan has been: Chairman of the Chemistry Department, 1982–86; Vice-Dean of the Faculty of Arts and Science, 1975–77; Vice-President, 1979–80, and President, 1986–88. Prof. Tarhan has also been President of the Eastern Mediterranean University, 1988–91. In addition, Prof. Tarhan has been Visiting Professor at the University of East Anglia, UK, and at the McNeil Pharmaceutical, Philadelphia, USA.

Offices and Assignments: Within IUPAC, Prof. Tarhan has, since 1988, been a Member (National Representative) of the Commission on Physical Organic Chemistry. He is also a member of the Turkish Chemical Society and, currently, is a member of the Scientific Commission of the 35th IUPAC Congress.

Prof. Tarhan's research interests are: acidity functions, kinetics and mechanisms of electrophilic aromatic substitution reactions, natural products (opium alkaloids), phytic acid determinations in food, and organic synthesis. He has published about 50 original research papers, reports and review articles in both English and Turkish.

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *PAC*.

Protocol for the design, conduct and interpretation of method-performance studies: revised 1994 (Technical Report)

Analytical methods have to be validated in order that they can stand up both to severe professional examination and possible legal challenge. The revised protocol incorporates the changes suggested following the experience gained by the international use of the First Protocol, *Pure Appl. Chem.* **60**, 855–864 (1988).

This report was prepared for publication by William Horowitz, Center for Food Safety and Applied Nutrition, Food and Drug Administration, Washington, DC 20204, USA, for the Interdivisional Working Party on Harmonization of Quality Assurance Schemes for Analytical Laboratories of the Analytical, Applied and Clinical Chemistry Divisions. The full details are published in Pure & Appl. Chem. ***67**, 331–343 (1995).*

Biocatalysis in non-conventional media: medium engineering aspects (Technical Report)

During the past decade, much progress has been made in the understanding of the various phenomena which govern biocatalysis in unconventional media. The factors which affect biocatalytic reactions and the activity and stability of biocatalysts in these reaction media are generally associated with the role of water and the need to keep biocatalysts in one active conformation. For the rational design of biocatalytic processes in the reaction media, discussed in this review, some basic rules have been formulated. These rules may serve as basic tools for future optimization of biocatalysis in non-conventional media and for engineering media for synthetic purposes.

This report was prepared for publication by M. H. Vermuë and J. Tramper, Food and Process Engineering group, Wageningen Agricultural University, PO Box 8129, Wageningen, Netherlands, for the Commission on Biotechnology of the Applied Chemistry Division. The full details are published in Pure & Appl. Chem. ***67**, 345–373 (1995).*

Recommended terminology for the description of carbon as a solid (IUPAC Recommendation 1995)

This document deals with the recommended terminology for the description of various solid forms of carbon used in science and technology of carbon and graphitic materials. The glossary also contains terms describing related materials, such as precursors for the production of carbon materials, and the processes used in their production. In all, 114 terms are defined, and comments and cross-references are included where appropriate.

Prepared for publication by E. Fitzer[1], K.-H. Köchling[1], H. P. Boehm[2] and H. Marsh[3] ([1]Institut für Chemische Technik der Universität Karlsruhe, Kaiserstrasse, Karlsruhe, Germany;[2] Institut für Anorganische Chemie der Universität München, Meiserstrasse, München, Germany; [3]Department of Geology, Southern Illinois University, Carbondale, IL 62901, USA) for the Sub-

committee on Terminology of Carbon SC-1, Commission on High Temperature and Solid State Chemistry of the Inorganic Chemistry Division. The full details are published in Pure & Appl. Chem. ***67**, 473–506 (1995).*

Selectivity coefficients for ion-selective electrodes; recommended methods for reporting $K^{pot}_{A,B}$-values (Technical Report)

The limitations of the Nicolsky–Eisenman (N-E) equation for the determination of potentiometric selectivity coefficients, $K^{pot}_{A,B}$, were critically evaluated in terms of $K^{pot}_{A,B}$-values for ions of unequal charge, non-Nernstian behaviour of interfering ions and activity dependence of $K^{pot}_{A,B}$. The reasons for the activity dependence of $K^{pot}_{A,B}$ and for nonequalities of values depending on the method employed have been elucidated. Also, when ions of different charge were involved, $K^{pot}_{A,B}$-values obtained were found to be either unrealistically large or small depending upon whether the ion of higher charge was considered as a primary or an interfering ion. On the basis of these considerations, new approaches including the matched potential method, independent of the N-E equation, are recommended for the determination of $K^{pot}_{A,B}$.

Prepared for publication by Yoshiso Umezawa[1], Kayoko Umezawa[2] and Hitoshi Sato[3] ([1]Department of Chemistry, University of Tokyo, Hongo, Tokyo, Japan; [2]Department of Chemistry, University of Tokyo, Komaba, Tokyo, Japan; [3]Department of Chemistry, Hokkaido University, Sapporo, Japan) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are published in Pure & Appl. Chem. ***67**, 507–518 (1995).*

Guidelines on nuclear magnetic resonance computerized databases (IUPAC Recommendation 1995)

With the widespread use and availability of computers for the acquisition and storage of NMR spectra, particularly proton and carbon spectra, it is evident that assembly and distribution of computer-readable NMR databases are desirable. To maximize the utility of such efforts, it is important to define a standardized format for information exchange and guidelines for information to be included in such databases. An equally important concern is the need for NMR databases, indeed, all databases of measured spectra, to include information which will allow potential users to determine the quality of the spectra. In 1984, a workshop on the subject of computerized databases, held in the National Bureau of Standards (NIST) of the United States, concluded that a consensus body such as IUPAC should be responsible for creating the necessary guidelines.

The present document is the result of the deliberations of the IUPAC Working Party on NMR computerized databases.

Prepared for publication by C. L. Wilkins, University of California, Riverside, CA 92521, USA, for the Working Party on Computerized NMR Databases in the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are published in Pure & Appl. Chem. ***67**, 593–596 (1995).*

Classification and chemical characterization of Immobilized enzymes (Technical Report)

Immobilized enzymes are becoming increasingly popular as reusable, selective analytical chemical reagents in solid-phase flow-through chemical reactors, as membranes in sensors and as films in dry reagent kits. Classification of such reagents must encompass the properties of the original enzyme, the type of support used and the methods of support activation and enzyme attachment. Important characteristics of an immobilized enzyme, *vis à vis* the enzyme in solution, for example, apparent activity, stability and lifetime must also be reported.

Prepared for publication by P.J. Worsfold, Department of Environmental Sciences, University of Plymouth, Plymouth, Devon PL4 8AA, UK, for the Commission on General Aspects of Analytical Chemistry of the Analytical Chemistry Division. The full details are published in Pure & Appl. Chem. ***67**, 597–600 (1995).*

Catalytic methods of analysis: characterization, classification and methodology (Technical Report)

Analytical methods based on the measurement of temporal changes in the concentration of certain components of suitable chemical reaction systems are varied, differing both methodically and in their application. This report, presents a classification of kinetic methods based on the chemistry of the reaction employed.

Catalytic determinations are the most widely used of the kinetic methods. The field of catalytic methods includes the methods of determination of trace concentrations of metal ions, anions and of many organic substances. Detectability at low levels with high sensitivities are recognized as major advantages of catalytic determinations. Selectivity, on the other hand, can be considered as a limitation to the practical application of these determinations.

Prepared for publication by H. Müller, Department of Chemistry, Martin-Luther-Universität, Halle, D06120, Germany, for the Commission on General Aspects of Analytical Chemistry of the Analytical Chemistry Division. The full details are published in Pure & Appl. Chem. ***67**, 601–613 (1995).*

Speciation of lead in environmental and biological samples (Technical Report)

The speciation of lead in environmental and biological samples is reviewed. After a brief outline of the occurrence, chemical transformations and impact of lead species, attention is focused on the various aspects of the analytical chemistry of lead speciation. Sampling, storage and pretreatment methods for water, air, solid and biological samples are discussed before an assessment of currently available analytical techniques and lead speciation schemes is made. Attempts have been directed towards critically choosing the most significant contributions to this subject, to assist the analytical chemist in the selection of the most suitable approaches to lead speciation and to provide a guide to the relevant literature.

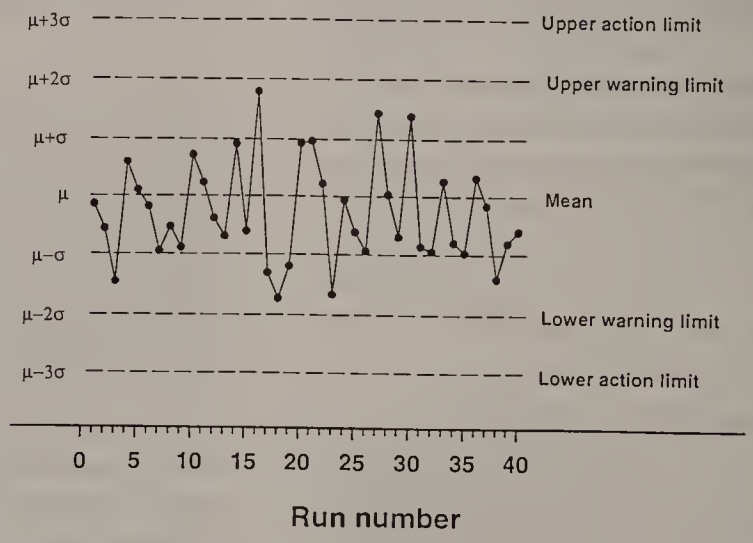
Prepared for publication by D. C. Baxter and W. Frech, Department of Analytical Chemistry, Umeå University, S-901 87 Umeå, Sweden, for the Commission on Microchemical Techniques and Trace Analysis of the Analytical Chemistry Division. The full details are published in Pure & Appl. Chem. ***67****, 615–648 (1995)*.

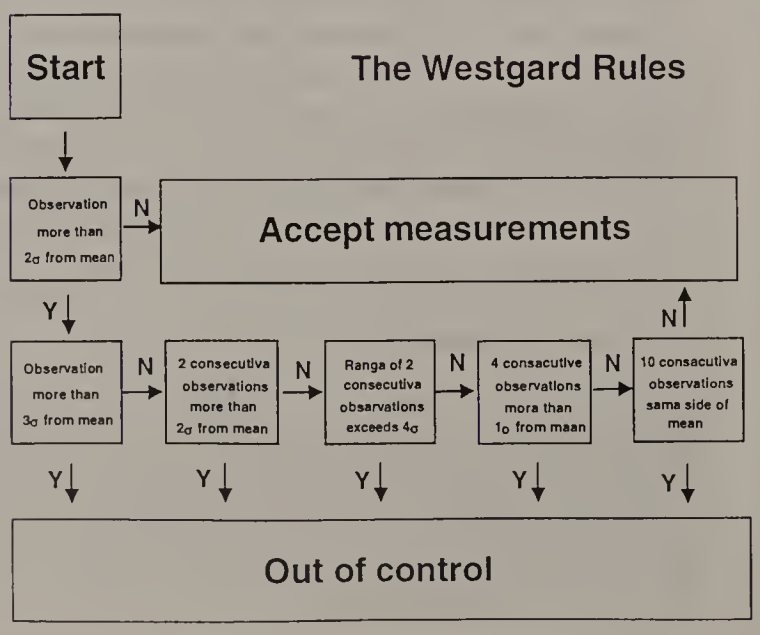
Harmonized guidelines for Internal quality control in analytical chemistry laboratories (Technical Report)

ISO, IUPAC and AOAC INTERNATIONAL have co-operated to produce agreed protocols on the *Design, Conduct and Interpretation of Collaborative Studies*, and on the *Proficiency Testing of (Chemical) Analytical Laboratories*. The working group that produced these protocols was asked to prepare guidelines on the internal quality control of data produced in analytical laboratories. Such guidelines would have to outline minimum recommendations to laboratories producing analytical data on the internal quality control procedures to be employed.

Prepared for publication by M. Thompson[1] and R. Wood[2] ([1]Department of Chemistry, Birkbeck College, London WC1H 0PP, UK;[2] MAFF Food Science Laboratory, Norwich Research Park, Colney, Norwich NR4 7UQ, UK) for the Interdivisional Working Party for Harmonization of Quality Assurance Schemes for Analytical Laboratories of the Analytical, Applied, Clinical, Inorganic and Physical Chemistry Divisions. The full details are published in Pure & Appl. Chem. ***67****, 649–666 (1995)*.

Results from a system in statistical control





Statistical controls on variable data and a flow chart for deciding on the acceptability of one particular result (taken from *Harmonized Guidelines for Internal Quality Control in Analytical Chemistry Laboratories*).

Publications

Tables of Intensities for Infrared Calibrations

The IUPAC Commission on Molecular Structure and Spectroscopy (1.5) of the Physical Chemical Division was established in 1955. It was appreciated that there was a great need for an organization to establish internationally accepted calibration standards, nomenclature and terminology. Infrared wave number calibration standards were established by Commission 1.5 in 1961. These initial tables were revised and the wave number range extended from 600–4000 cm^{-1} to 1–4350 cm^{-1} in 1973, and were again revised in 1977. The values have been approved by the Interunion Commission on Spectroscopy of the International Council of Scientific Unions on which the International Unions of Astronomy and of Physics are also represented.

The situation concerning infrared intensity measurements is very different. No intensity standards have yet been published. Commission 1.5 recognized the necessity of such standards, so a Working Party on Secondary Standards for Intensity Measurements in Infrared Spectroscopy was established, directing it to give particular attention to measurements in the liquid phase.

The Working Party has now presented its results on four liquids: benzene, toluene, chlorobenzene and dichloromethane, which form the present volume.

The basic spectroscopic measurement is the transmittance, $t(\nu)$, of the sample. This is the ratio $(I(\nu)/I_o(\nu))$ of the monochromatic radiant power transmitted through the sample to that incident on the sample, after appropriate correction has been made for all losses other than absorption. These corrections for secondary radiation losses are complex and are discussed in detail in the references in the present volume.

The decadic absorbance, $A(\nu)$ is computed as:

$$A(\nu) = \log (I_o(\nu)/I(\nu)) = -\log t(\nu)$$

On the assumption of the Beer–Lambert law, several different quantities that describe the absorption intensity may be calculated from the absorbance.

In general, spectroscopists prefer to express infrared intensities in terms of the optical constants, $n(\nu)$ and $k(\nu)$, which are, respectively, the real and imaginary components of the complex refractive index $n^*(\nu)$:

$$n^*(\nu) = n(\nu) + ik(\nu).$$

The imaginary component is known as the absorption index and is given by:

$$k(\nu) = 2.303\, A(\nu)/4\, \nu\pi d$$

where d is the sample thickness expressed in units which are the inverse of ν, so that $k(\nu)$, like $A(\nu)$, is dimensionless. However, many spectroscopists who work with liquids prefer to use the molar (decadic) absorption coefficient E_m as a measure of absorption:

$$E_m(\nu) = A(\nu)/C\, d = 4\, \nu\pi\, k(\nu)/2.303\, C$$

where C is the molar concentration. The tables of intensities given in the present volume are listed as n, k and E_m. Following tradition, the path length is quoted in centimeters, and the molar concentration in mol L^{-1}. Thus, the values of E_m are given in L mol^{-1} cm^{-1}.

The choice of liquids investigated was determined by: their ready availability in high purity, their simple molecular structure which makes them amenable to a full force-field vibronic analysis, and the absence of conformational or hydrogen bonding equilibria which would have tended to give complex temperature-dependent effects in the intensities and profiles.

To encourage uniformity in the application of these standards in quantitative analysis, the authors have developed an algorithm which has been incorporated into a FORTRAN program IRYTRUE. This program is described in detail and an executable version accompanied the book on a diskette. The program has been tested over many years in several laboratories on a wide range of IBM compatible personal computers with the MS-DOS and OS/2* operating systems.

IRYTRUE excepts as input a file of experimental wave number-absorbance values for one or more of the standard calibration bands. It checks and corrects baseline displacements across the integration range of interest and then computes the E_m spectrum on the basis of its estimation of the path length and integrates the area under this E_m curve above a linear baseline between the ordinate values at the integration limits. This area in then ratioed to the corresponding area of the standard band, which is then stored.

A cell constant is calculated by multiplying the initial cell path length by the above ratio and a new set of E_m values is derived using this cell constant in place of the path length. This procedure is iterated until a constant value for the cell constant is achieved. This cell constant may then be used in place of the measured path length in subsequent analytical calculations. The Appendices of this book outline the use of three supplementary programs to be found on the diskette accompanying this volume.

Tables of Intensities for the Calibration of Infrared Spectroscopic Measurements in the Liquid Phase. *Prepared for publication by, J. E. Bertie, C. Dale Keefe and R. Norman Jones. Chemical Data Series No.40. Blackwell Science, Osney Mead, Oxford OX2 0EL, UK, 1995. Price GBP49.50, ISBN 0-86542-928-X.*

Provisional Recommendations

IUPAC seeks you comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional center requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most up-to-data list of the national/regional centers appears in this issue.

Basic terms in polymer science

The clear and unambiguous definition of basic terms in a field of science has special significance. Subsequent nomenclature must refer back to these basic terms and the greatest care is required in preparing and revising them. In 1974, the Commission on Macromolecular Nomenclature published a document entitled **Basic definitions relating to polymers**, *Pure & Appl. Chem.* **40**, 479–491 (1974). These definitions have been the foundation of the Commission's work and have spawned a number of further documents on nomenclature.

The vast majority of terms in the basic document serve their purpose well. Progress in polymer science and the need for new definitions, the proper wording of which would have contradicted some of the basic terms, made it increasingly apparent that some changes were required in the basic terms. Approximately 20 years since the appearance of the first document, the Commission on Macromolecular Nomenclature now issues a revised and enlarged set of basic terms. The new glossary of terms has been formulated by the commission with the additional input and aid of several well-known researchers and journal editors. It provides 135 definitions and 187 defined terms.

Comments on these recommendations are welcome and should be sent by November 30th 1995 to:

Prof. R. F. T. Stepto, Polymer Science and Technology Group, Manchester Materials Science Center, University of Manchester and UMIST, Grosvenor Street, Manchester M1 7HS, UK

What happens to polymers after their initial use affects us all.

Definitions of terms relating to degradation, aging, and related chemical transformations of polymers

Chemical reactions of polymers are very important from the point of view of chemical modifications of polymers to improve properties and changes in structure and physico-chemical properties in the course of synthesis, processing, applications or the action of chemicals and micro-organisms.

However, terminology in this field has developed in an *ad-hoc* basis in different professional communities. This document presents therefore an alphabetical list of terms relating to degradation, aging and related chemical transformation of polymers, defining a self-consistent terminology for this field which will aid communication and help to avoid confusion.

Some of the general definitions are modified by one or more prefixes or adjectives describing type or cause. Definitions of basic terms such as aging, degradation and stability have notes appended relating to specific causes. For example, definitions of different types of aging, such as artificial, cosmic, ground or radiation aging, are covered by notes under the general term 'aging'. Adjective-modified terms that are frequently used by themselves are defined separately; biodegradation, photostabilizer, and chain-terminating antioxidant are typical examples. An index is appended for the readers convenience.

Comments on these recommendations are welcome and should be sent by November 30th 1995 to:

Prof. K. Hatada, Department of Chemistry, Faculty of Engineering Science, Osaka University, Toyonaka, Osaka 560, Japan

Addresses of National/Regional Centres

If you would like to comment on provisional recommendations please write to your nearest national/regional center requesting a copy of the full report. Copies are not available from the Secretariat. The most up-to-date list of national/regional centers is shown below:

Argentina

Dr Y. Salum,
Director, Indústria y Química,
Asociación Química Argentina,
Sánchez de Bustamante 1749,
Buenos Aires,
Argentina

Asia (Australia, Bangladesh, Hong Kong, Indonesia, Iraq, Korea, Malaysia, Nepal, Philippines Singapore, Sri Lanka, Thailand)

Prof. Sang up Choi,
c/o Korean Chemical Society,
35 5 – KA Anam Dong,
Sungbuk-ku,
Seoul 136-075,
Republic of Korea

Canada

Prof. J. ApSimon
Director of Research, Dean,
Faculty of Graduate Studies and Research,
Room 1525, Dunton Tower,
Carleton University,
Ottawa,
Canada K1S 5B6

China/Taiwan

Prof. Ta-Shue Chow,
Institute of Chemistry,
Academia Sinica,
Nankang,
Taipei,
Taiwan 11529

Czech Republic

Dr J. Kahovec,
Institute of Macromolecular Chemistry,
Academy of Sciences of the Czech Republic,
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Czech Republic

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Prof. Françoise Rouquérol,
Laboratoire de Physico-Chimie des Interfaces,
Université de Provence,
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Germany

Dr Eva E. Wille,
Journal Department Manager,
VCH Verlagsgesselschaft,
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Germany

Hungary

Hungarian National Committee for IUPAC,
Institute for General and Analytical Chemistry,
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Hungary

India

Dr V. C. Vora,
Indian National Science Academy,
Bahadur Shah Zafar Marg,
New Delhi 110002,
India

Italy

Prof. G. Scorrano,
President, Società Chimica Italiana,
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Viale Liege 48,
Italy

Japan

Dr A. Nakanishi,
Executive Director,
Chemical Society of Japan,
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Chiyada-ku,
Tokyo 101,
Japan

The Netherlands

Ir. E. J. Ryck van der Gracht,
Koninklijke Nederlandse Chemische Vereniging,
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The Netherlands

People's Republic of China

Prof. X. Qiu,
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POB 2709,
Beijing,
China

Poland

Prof. O. Achmatowicz
Pharmaceutical Research Institute,
Rydygiera 8,
01-793 Warsaw,
Poland

Russia

Prof. G. B. Bokij
Russian Academy of Sciences,
National Committee of Russian Chemists,
19 Kosygin Street,
117975 Moscow,
Russia.

Republic of South Africa

Prof. J. R. Bull
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University of Cape Town,
Rondebosch 7700,
Republic of South Africa

Sweden

Dr K. Samuelsson,
Svenska Nationalkommittén för kemi,
Wallingatan 26B,
S-11 24 Stockholm,
Sweden

UK

Dr A. D. McNaught,
The Royal Society of Chemistry,
Thomas Graham House,
Science Park, Milton Road,
Cambridge CB4 4WF
UK

USA

Dr Mary E. Scanlan,
Journals Department,
American Chemical Society,
2540 Olentangy River Road,
PO Box 3330 Columbus,
Ohio 43210,
USA

75th Anniversary Celebrations in the Far-East

To celebrate the 75th anniversary of IUPAC, a symposium entitled 'Chemistry for Life' was held on 12 October 1994 at the National Central Library, Taipei, Taiwan, ROC. The local organizers of this symposium were the Chemical Society located in Taipei and the meeting was sponsored by the National Science Council, Academica Sinica, China Technical Consultants, Inc., and Union Chemical Laboratories, ITRI.

The speakers were Prof. A. E. Fischli, President-Elect of IUPAC, Prof. Yuan T. Lee, Nobel Laureate in Chemistry 1986 and President of the Academia Sinica, and Dr Yoshikazu Ito, Chairman of Toray Industries, Inc., Japan.

Prof. Fischli introduced the audience to 'Chemistry and Industry', showing how chemistry is the central science spanning a multitude of other fields of scientific endeavour. This talk showed how the availability of capital and good ideas are necessary to produce successful consumer products. Focusing on the pharmaceutical industry, Prof. Fischli demonstrated the various economic and governmental forces which operate on pharmaceutical research departments and which can strongly influence the development of new therapeutic agents.

Subsequently, Prof. Lee showed how a combination of modern laser technology and molecular beams can be used to study chemical reactions which are of fundamental importance to the quality of the environment, 'Chemistry and the Environment'. Chemical kinetics plays a fundamental part in combustion processes and astrometrology; air pollution, acid rain and ozone-layer depletion are the result of chemical reactions. Classical chemical kinetics focuses on measurements of the rate of reaction and how this rate varies with bulk temperature and pressure. Modern chemical kinetics, on the other hand, focuses on the dependence of the rate on the amount of energy present in one reactant molecule and how the observed reaction rate varies with the amount of vibrational or rotational energy present in the interacting molecules.

Finally, Dr Yoshikazu Ito spoke about 'Chemistry for Life' stressing that for basic research the most important resource we possess are the young scientists engaged in this work. Chemical industry must respond to the changing imperatives of human society and must nurture young creative researchers with fresh ideas and challenging spirits.

After these seminars, there was a regional meeting of COCI where Dr Kazuo Saito (Japan) introduced the subject of the IUPAC CHEMRAWN Conferences and Dr Min Cho Chon (Korea) outlined the preparations for CHEMRAWN IX (1–5 September 1996, Seoul Korea).

Dr Nukada (COCI) presenting one of the competition winners with their prize.

The Japanese Company Associates celebrated the 75th Anniversary of IUPAC with a meeting in Tokyo, 6 November 1994. Indeed, for this celebration, cosponsored by the Chemical Society of Japan, Japan Chemical Industry Association, Society of Chemical Engineers and the Association for the Progress of New Chemistry, the Company Associates participated in a writing competition for school children.

A competition was held to find the best essay written on a preset subject 'Our Life and Dreams of Chemistry'. The subject matter for the more than four thousand entries received by the secretariat ranged over new materials, environmental improvements, contamination of drinking water.

Climate change

In Rio de Janeiro, in 1992, the world's leader started thinking about how to limit the threat of global warming caused by the increasing presence of greenhouse gases in the Earth's atmosphere. For a few months, the treaty signed in Rio gave the world the impression that something was being done to safeguard our environment. Unfortunately, although there was, at that time, a great deal of evidence for man's deleterious impact on the atmosphere, a great many scientists still supported the idea that the observed upward trends in global temperatures were not abnormal and that there is no greenhouse effect, and that atmospheric scientists who contend the contrary are really only observing natural fluctuations which modulate the surface temperature of the Earth.

However, subsequent to this meeting more and more evidence has been accumulated that global warming is a reality. There is, for example, a global recession of

glaciers – only a very small percentage of the Earth's glaciers have advanced in the last few years. It is believed that 10–20% of the Earth's mountain glaciers have melted in the last century. Although the average temperature over the whole of Antarctica has not risen in a statistically significant manner in the recent past, local temperatures over parts of Antarctica have risen dramatically, 2.5 °C over the Antarctic Peninsular in the last 40 years. This heating has resulted in large pieces, many thousands of square kilometers, of the ice shelf breaking away from the southern continent.

Such recent observations are now beginning to convince some of the earlier skeptics that anthropogenic effects on the atmosphere are real.

Figure 1 shows the combined land, air and sea surface temperature (°C) for 1860–1994, relative to the period 1951–80 (an average of the temperatures is taken as a point of origin in any comparison). The data point for 1994 is provisional and has not yet been fully analysed, however, 1994 was the third or fourth warmest year on record. The solid curve was obtained by filtering the data to highlight decade and longer-term trends.

It is clearly seen in Fig. 1 that measured global temperatures have been falling since 1990. However, before we start congratulating ourselves that measures taken to limit greenhouse gas emissions are starting to have a noticeable effect, it needs to be pointed out that this observed fall in temperature is believed to be due to volcanic activity. In 1991, Mt. Pinatubo in the Philippines erupted spectacularly. Indeed, it was one of the biggest eruptions in recent history. The amount of solid debris thrown into the atmosphere by this eruption reduced, by absorption and reflection, the amount of solar radiation reaching the Earth's surface. It is believed that the reduction of about 0.2 °C in global temperatures from 1991 to 1992 was partly due to this event and will henceforth be of diminishing importance.

The origins of the greenhouse gases are many and varied, however, the combustion and partial combustion of fossil fuels are man's main contribution to global warming. However, the process is not a simple one, when fossil fuels are burnt, a number of different gases are emitted. The largest product, by volume, is CO_2 with SO_2 being a smaller constituent. Unlike CO_2, SO_2 is chemically reactive and enters a variety of chemical processes in the atmosphere. Under dry conditions, the emitted SO_2 ends up, after 2–3 days, as small (0.01–0.1 μm) particles or droplets of sulfates. Such particles are termed aerosols. Aerosols do occur naturally, e.g. dust, sea salt and soot. However, anthropogenic emissions of SO_2 increase significantly the amount of aerosols present in the atmosphere. Under wet condition, the SO_2 rapidly produce relatively large droplets of sulfates, usually ammonium sulfate, which again condense into aerosol droplets or particles.

Thus, emissions of SO_2 affect the natural population of aerosols in the atmosphere, they increase the total concentration of aerosols present and through the wet pathway, they produce larger aerosol particles. Like natural aerosols, the sulfate aerosols have a lifetime in the atmosphere of about 10 days – they are washed out by rain, and settle under the influence of gravity.

The importance of aerosols in the atmosphere is that they reduce the amount of sunlight reaching the Earth's surface, i.e. like volcanic ash and dust they scatter some of the incoming solar radiation. Consequently, they operate in the opposite manner to the greenhouse gases in the atmosphere which trap radiation and heat the atmosphere. The aerosols scatter incoming radiation and reduce the heating of the atmosphere. It is estimated that the total 'radiative forcing' caused by anthropogenic aerosols is between –0.3 and –2.0 Watts per meter squared (W m^{-2}). There is a large uncertainty because of the lack of reliable observations of aerosol concentration and uncertainty about their origins.

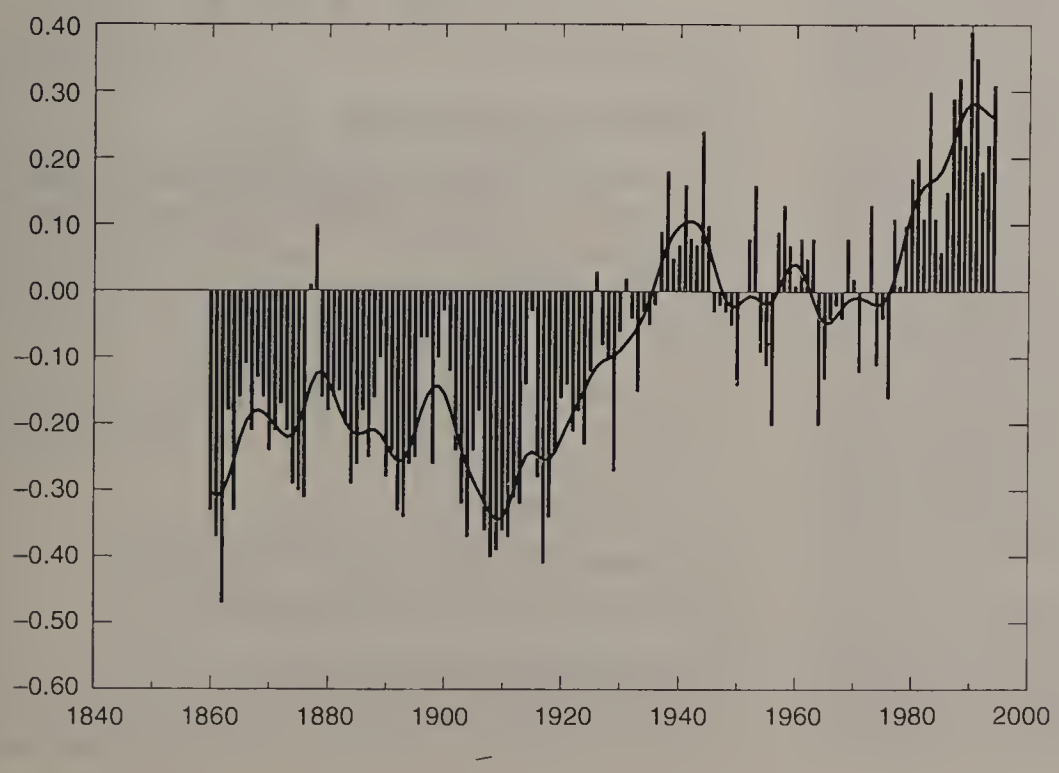

Figure 1. Combined land air and sea surface temperatures relative to 1951–80 averages.

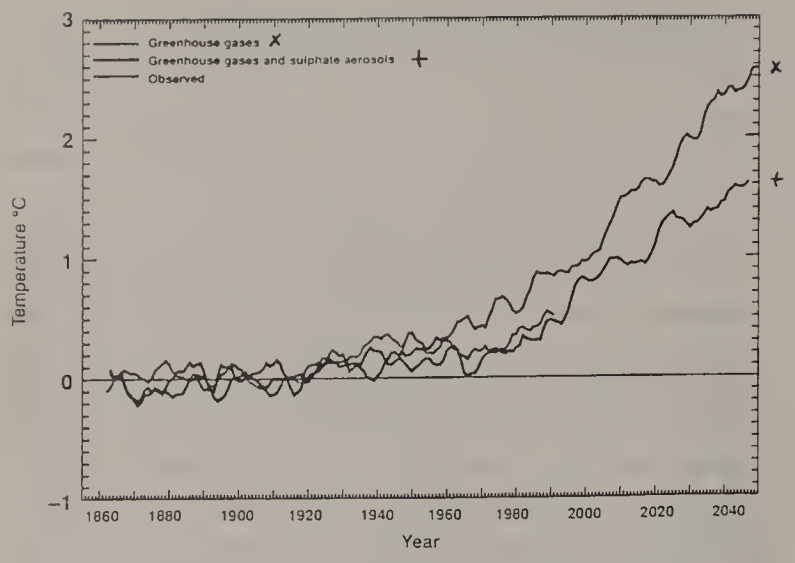

Figure 2. Predicted (1860–2050) and observed (1860 to present-day) surface air temperature changes (°C).

Carbon dioxide is estimated to have an atmospheric lifetime of between 50 and 200 years and is nearly uniformly distributed within the atmosphere, aerosols are normally found down wind of industrialized nations. Pre-industrial atmospheric concentrations of CO_2 were about 280 ppm, current values are about 355 ppm with anthropogenic emissions adding about 3 ppm per annum. It is estimated that the radiative forcing, i.e. the energy trapped by this greenhouse gas, is about 2.5 W m^{-2}.

The Hadley Center for Climate Prediction and Research was established in the early 1990s as an offshoot of the Meteorological Office, Bracknell, UK. They have recently issued a report, *Modelling Climate Change 1860–2050*, which details the results of their extensive computer modelling of the atmosphere and how it will evolve in the next century. These computer modellers have included in their calculations two factors of human origin, namely the emission of greenhouse gases and the presence of sulfate aerosols. The influence of greenhouse gases on global temperatures has been investigated in other modelling studies and the results of the present studies are in agreement with previous work. The presence of aerosols which contribute to the global temperature in the opposite sense from the greenhouse gases is an innovation.

A General Circulation Model (containing representations of the atmosphere, oceans, ice and vegetation) has been able to replicate in broad terms the observed slow rise in global temperatures since the middle of the last century. If greenhouse gases alone were influencing climate we would expect global temperatures to have risen by between 0.6–1.3 °C over the last century (Intergovernmental Panel on Climate Change, IPCC, 1990). By taking into account the contribution of aerosols to the global temperature, the Hadley Center model simulates a rise in temperature close to the observed 0.5 °C over the last century.

The experiment was extended to 2050 using a 'non-interventionist' emission scenario similar to that prepared by IPCC. The model predicts a long-term increase in global temperatures slightly in excess of 0.2 °C per decade, which is twice the rate which many of the more sensitive ecosystems can tolerate or adjust to (analysis of the temperature record of the last 1000 years has revealed that ecosystems can tolerate and adapt to temperature changes of order 0.1 °C per decade). When the cooling effects of the atmospheric sulfate aerosols are removed, the model predicts a warming of 0.3 °C per decade, which is consistent with previous estimates from IPCC. Figure 2 displays these predicted global temperature changes.

It is to address some of these serious concerns that the First Conference of the parties to the Framework Convention on Climate Change was held in Berlin, Germany, 27 March – 7 April 1995. This was the first serious test of the Rio Convention. Although the problem of greenhouse emissions is central to global warming, it is however, not in a governments gift to limit such emissions by legislation. Any such limitations will have a profound effect on the economy of both developed and developing industrial countries and consequently be of considerable importance to governments who a struggling to move their economies out of the recent recession.

The Hadley Center's calculations were undertaken on a CRAY C90 and required three months of computational time. For further interest in the Hadley Center, please contact:

Dr D. A. Bennetts, Research Co-ordinator
Hadley Center, Meteorological Office
London Road, Bracknell
Berks. RG12 2SY, UK
Tel.: + 44 (1344) 856653
Fax: + 44 (1344) 854898
Internet: dabennett@meto. govt.uk

IUPAC colleagues deceased

Poland Prof. T. Plebanski (20th September 1994) – Commission on Physicochemical Measurements and Standards (1961–83).

Names and addresses

Full details (names, addresses, telephone/telex/Fax: numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* **15**, 215–227 (1993). The IUPAC Secretariat have been notified of the following changes:

Prof. Alan M. Bond, Monash University, Clayton, Victoria 3168, Australia. Tel.: (61) 39905 1338, Fax: (61) 39905 4597, E-mail: a.bond@sci.monash.edu.au

Dr Anders Kallner, E-mail: anka@cc.ks.se

Dr Larry Fox, E-mail: larryfox@amoco.com

Dr G. M. Rosenblatt, E-mail: grosenblatt@Csa2.lbl.gov

IUPAC 1994

Maurice Williams

Each year, IUPAC Executive Secretary Dr Maurice Williams prepares a report on IUPAC activities for the International Council of Scientific Unions (ICSU). This is his report for 1994.

For IUPAC, 1994 was the 75th anniversary of its foundation. As a non-General Assembly year, the business of the Union was conducted through meetings of the Executive Committee (Oxford, April) and the Bureau (Antwerp, September). Bulgaria and Nigeria ceased to be Members of the Union because of arrears in their annual subscriptions.

To celebrate the 75th anniversary, a series of national and regional activities on the theme *Chemistry for Life* was co-ordinated by the Committee on Chemistry and Industry (COCI). The aim was to promote chemistry and its image among high-school students, teachers, and the general public, through lectures, poster competitions, magazines and books, and television programs. Some 14 countries were involved. Regional events were held in Europe (Brussels), North-West Pacific Rim (Taiwan), and North America (Washington, DC), with contributions from Nobel prize winners, chief executive officers from industry, and government ministers concerned with ecology, economy, and education.

Another landmark was reached with publication of *History of IUPAC: 1919–87*. This book was the culmination of several years of research by Mr R. W. Fennell, and the material chosen illustrates, sometimes at length, the difficulties, political, financial, and technical, which have arisen as well as the successes that have been achieved, the bright ideas, and the administrative peculiarities.

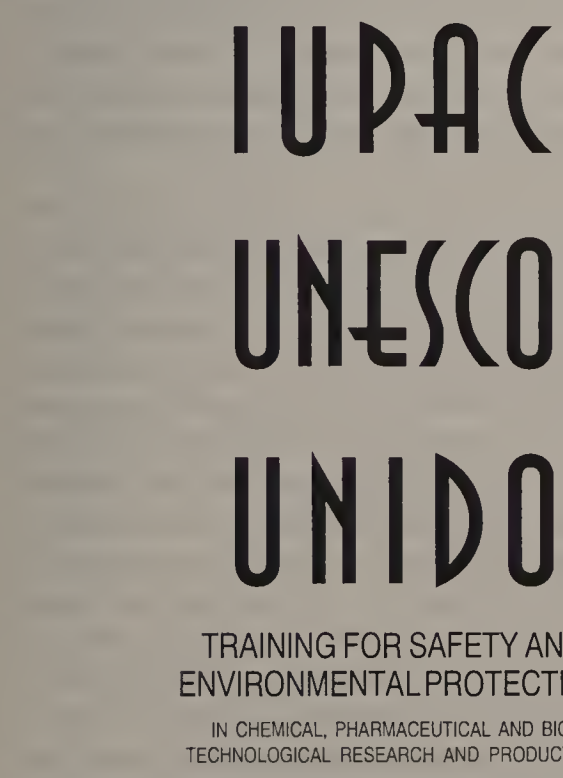

Fig. 1. The IUPAC–UNESCO–UNIDO Training Programme, one of the great successes of international collaboration.

A particular success was the fruitful co-operation between UNESCO and IUPAC. UNESCO is assisting in running the CHEMRAWN programme, as well as supporting projects to be carried out by the Divisions in those areas which are considered to be of high priority by UNESCO. Already in the 1994–95 biennial budget of UNESCO, funding was made available for a few projects to be carried out by the Union in 1995. In addition, the planning of the IUPAC input in the framework of the 1996–97 UNESCO budget has started. The co-operation continued to include the training programme for safety and environmental protection in chemical production, in which the IUPAC partner is COCI.

A long-standing problem for IUPAC has been to make recommendations on names and symbols for the transfermium elements. Interim systematic names had been recommended (1979), and a Transfermium Working Group (TWG) was set up (1986) under the joint auspices of IUPAC and IUPAP. The TWG's conclusions on criteria that must be satisfied for the discovery of a new chemical element to be recognized and on discovery of the transfermium elements, were duly endorsed by the two Unions. These conclusions were considered last year by the IUPAC Commission on Nomenclature of Inorganic Chemistry, whose recommendations in respect of the transfermium elements were accepted by the Bureau and published. They included a principle that an element should not be named after a living person, and took account of the suggestions of the three laboratories involved in the choices for names. The recommendations provoked strong criticism from some parts of the world.

In 1986, IUPAC launched an Affiliate Membership Programme in order to maximize the participation of individual chemists throughout the world in its affairs. The number of Affiliates has declined in the last few years, and a critical review of the Programme was undertaken in 1994 by a small group on behalf of the Bureau. Continuation of AMP was advocated for the biennium 1996–97, subject to steps being taken to ensure its future viability and growth.

As a result of further discussions on restructuring of the scientific activities of the Union in high-priority areas, the pool of 18 Titular Member positions operating during 1994–95 will be enlarged to 24 for 1996–97. A number of these positions were allocated to the Divisions for innovative activities, and others to projects proposed by Bureau members. A start on the designated projects will be made at the General Assembly in 1995. The successful project requests include oil spill clean-up and remediation, remediation of heavy ele-

ment contaminated sites, polymers and the environment, and environmental safety assessment of agrochemicals. Furthermore, discussions on restructuring the divisional framework of IUPAC were extended to include focusing the scientific efforts more in the direction of the role of chemistry in the study of the environment, health, materials, and biochemistry.

A review of IUPAC activities in environmental chemistry, prepared by Prof. J. G. Calvert, was presented and well received by the Bureau. The document is being extended prior to dissemination. At the WHO International Conference on Chemical Safety (Stockholm), it was resolved to establish an Intergovernmental Forum on Chemical Safety. An *ad hoc* group of non-governmental organizations, including IUPHAR, IUTOX, and IUPAC, offered their technical support to the work of the Forum. In the case of IUPAC, it is envisaged that such technical expertise might be provided through COCI.

Progress in the planning for CHEMRAWN IX reached the stage when official sponsorship could be granted by IUPAC. The subject was confirmed as *Sustainable Production, Use and Disposal (including Recycling) of Materials*, and the Conference is regarded as a follow-up to CHEMRAWN VI (Tokyo, 1987), with four main orientations of the subject to be treated in parallel sessions: energy, transportation, communication, and construction (building materials). It is scheduled to take place in Seoul during 96.09.01–06, in conjunction with the 50th anniversary of the Korean Chemical Society. The technical proceedings from CHEMRAWN VII (Baltimore, 1991) – *Chemistry of the Atmosphere: Its Impact on Global Change* – were published as a monograph in the IUPAC series *Chemistry for the 21st Century*. Also, more of the scientific papers presented at CHEMRAWN VIII (Moscow, 1992) – *Chemistry and Sustainable Development: Towards a Clean Environment, Zero Waste and Highest Energy Efficiency* – were published in a second issue of the new journal *Chemistry and Sustainable Development*.

In a response to criticism that the biennial IUPAC Congresses were now outmoded, a position paper was developed with the aim that they should constitute a central international event in the world of chemical research. A drastic change in content, format, and scientific planning is envisaged, under the name *Frontiers in Chemistry*. Rather than continue the present practice of including all main branches of chemistry, there will be coverage of only two to four branches, focusing on interdisciplinary topics at the frontiers of modern chemistry. Greater involvement of IUPAC bodies is foreseen in planning, shaping, and executing the scientific programme. The changes are to be introduced gradually for 1997, with full implementation in 1999. Furthermore, for 1997 IUPAC agreed to locate its General Assembly and Congress, back-to-back, in Rio de Janeiro, the first occasion these events have been scheduled for the southern hemisphere.

Three IUPAC projects were funded with ICSU support in 1994, namely, *Education in Materials Science, Quality Assurance,* and *Workshop on QSARs*. Of these, significant progress was made in defining a suitable programme in materials science and engineering for emerging countries. At a workshop during the 1994 International Symposium on Macromolecules (Akron, Ohio), it was decided to concentrate efforts on Africa. A further meeting is planned in conjunction with the International Conference on Chemistry in Africa (Accra, July August).

The Quality Assurance project was run by three relevant IUPAC bodies, through working groups, to improve the quality and reliability of work undertaken in analytical chemical laboratories. The groups met separately (Delft, Barcelona, and Buenos Aires), and four documents and a substantial monograph have been produced or are in preparation. Quantitative Structure Activity Relationships (QSARs) are used to estimate the rates of certain chemical processes, when there is a paucity of experimental data. A workshop was held at Belgirate (Italy), in collaboration with the Commission on Water Chemistry, to discuss the present state of knowledge regarding biodegradative transformation pathways and methods available to predict rates of biotransformation of organic compounds. Recommendations were made on the use of QSARs for predicting the course of biodegradative transformation pathways under realistic environmental circumstances.

Fig. 2. Industrial conditions in many developing countries necessitates that the local safety officers be given the very best experience possible.

Appendix

The following nomenclature reports (IUPAC Recommendations 1994) were published during the year:

1 Commission on Thermodynamics, 'Standard quantities in chemical thermodynamics: Fugacities, activities, and equilibrium constants for pure and mixed phases', *Pure Appl. Chem.* **66**, 533–552 (1994).
2 Commissions on Electrochemistry and Electroanalytical Chemistry, 'Terminology and conventions for microelectronic ion-selective field effect transistor devices in electrochemistry', *Pure Appl. Chem.* **66**, 565–569 (1994).
3 Commission on Molecular Structure and Spectroscopy, 'Symbols for fine and hyperfine structure parameters', *Pure Appl. Chem.* **66**, 571–576 (1994).
4 Commission on High Temperature and Solid State Chemistry, 'Definitions of terms relating to phase transitions of the solid state', *Pure Appl. Chem.* **66**, 577–594 (1994).
5 Commission on Analytical Nomenclature, 'Nomenclature for presentation of results of chemical analysis', *Pure Appl. Chem.* **66**, 595–608 (1994).
6 Commissions on Analytical Nomenclature and General Aspects of Analytical Chemistry, 'Nomenclature in laboratory robotics and automation', *Pure Appl. Chem.* **66**, 609–630 (1994).
7 Commission on Macromolecular Nomenclature, 'Structure-based nomenclature for irregular single-strand organic polymers', *Pure Appl. Chem.* **66**, 873–889 (1994).
8 Commission on Quantities and Units in Clinical Chemistry and IFCC Committee on Quantities and Units, 'Quantities and units for electrophoresis in the clinical laboratory', *Pure Appl. Chem.* **66**, 891–896 (1994).
9 Commission on Quantities and Units in Clinical Chemistry and IFCC Committee on Quantities and Units, 'Quantities and units for centrifugation in the clinical laboratory', *Pure Appl. Chem.* **66**, 897–907 (1994).
10 Commission on Quantities and Units in Clinical Chemistry and IFCC Committee on Quantities and Units, 'Application of IUPAC–IFCC recommendations on quantities and units to WHO biological reference materials for diagnostic use', *Pure Appl. Chem.* **66**, 909–913 (1994).
11 Commission on Physical Organic Chemistry, 'Glossary of terms used in physical organic chemistry', *Pure Appl. Chem.* **66**, 1077–1184 (1994).
12 IUPAC–IUBMB Joint Commission on Biochemical Nomenclature, 'Recommendations for nomenclature and tables in biochemical thermodynamics', *Pure Appl. Chem.* **66**, 1641–1666 (1994).
13 Commission on Colloid and Surface Chemistry including Catalysis, 'Thin films including layers: Terminology in relation to their preparation and characterization', *Pure Appl. Chem.* **66**, 1667–1738 (1994).
14 Commission on Electrochemistry, 'Impedances of electrochemical systems: Terminology, nomenclature and representation – I: Cells with metal electrodes and liquid solutions', *Pure Appl. Chem.* **66**, 1831–1891 (1994).
15 Commission on High Temperature and Solid State Chemistry, 'Nomenclature and terminology of graphite intercalation compounds', *Pure Appl. Chem.* **66**, 1893–1901 (1994).
16 Commissions on Analytical Nomenclature and General Aspects of Analytical Chemistry, 'Nomenclature of interlaboratory analytical studies', *Pure Appl. Chem.* **66**, 1903–11 (1994).
17 Commission on Nomenclature of Inorganic Chemistry, 'Names and symbols of transfermium elements' *Pure Appl. Chem.* **66**, 2419–2421 (1994).
18 Commission on Atomic Weights and Isotopic Abundances, 'Atomic weights of the elements 1993', *Pure Appl. Chem.* **66**, 2423–2444 (1994).
19 Commission on Electrochemistry, 'Terminology and notations for multistep electrochemical reaction mechanisms', *Pure Appl. Chem.* **66**, 2445–2450 (1994).
20 Commission on Macromolecular Nomenclature, 'Graphic representations (chemical formulae) of macromolecules', *Pure Appl. Chem.* **66**, 2469–2482 (1994).
21 Commission on Macromolecular Nomenclature, 'Basic classification and definitions of polymerization reactions', *Pure Appl. Chem.* **66**, 2483–2486 (1994).
22 Commissions on General Aspects of Analytical Chemistry and Thermodynamics, 'Nomenclature of thermometric and enthalpimetric methods in chemical analysis', *Pure Appl. Chem.* **66**, 2487–2492 (1994).
23 Commission on General Aspects of Analytical Chemistry, 'Classification and definition of analytical methods based on flowing media', *Pure Appl. Chem.* **66**, 2493–2500 (1994).
24 Commission on Analytical Nomenclature, 'Nomenclature for radioanalytical chemistry', *Pure Appl. Chem.* **66**, 2513–2526 (1994).
25 Commission on Electroanalytical Chemistry, 'Recommendations for nomenclature of ion-selective electrodes', *Pure Appl. Chem.* **66**, 2527–2536 (1994).
26 Commissions on Automation and Clinical Chemical Techniques and Analytical Nomenclature, 'Glossary of bioanalytical nomenclature – I: General terminology, body fluids, enzymology, immunology', *Pure Appl. Chem.* **66**, 2587–2604 (1994).

The following technical reports by IUPAC bodies were published during the year:

1 Commission on Biotechnology, 'Interrelations of chemistry and biotechnology – IV: Biochemical engineering in biotechnology', *Pure Appl. Chem.* **66**, 117–136 (1994).
2 Commission on Atmospheric Chemistry, 'Assessment of uncertainties in the projected concentrations of methane in the atmosphere', *Pure Appl. Chem.* **66**, 137–200 (1994).
3 Commission on Atomic Weights and Isotopic Abun-

dances, 'Reporting of stable hydrogen, carbon, and oxygen isotopic abundances', *Pure Appl. Chem.* **66**, 273–276 (1994).

4 Commission on General Aspects of Analytical Chemistry, 'Analyte isolation by solid phase extraction (SPE) on silica-bonded phases: Classification and recommended practices', *Pure Appl. Chem.* **66**, 277–304 (1994).

5 Commission on Radiochemistry and Nuclear Techniques, 'Applications of accelerator mass spectrometry in analysis of trace isotopes and elements', *Pure Appl. Chem.* **66**, 305–334 (1994).

6 Commission on Agrochemicals, 'Effects of storage and processing on pesticide residues in plant products', *Pure Appl. Chem.* **66**, 335–356 (1994).

7 Commission on Toxicology, 'Measurement of total nickel in body fluids: Electrothermal atomic absorption methods and sources of preanalytical variation', *Pure Appl. Chem.* **66**, 357–372 (1994).

8 Commission on Thermodynamics, 'Vapour-liquid equilibria in alkan-1-ol + *n*-alkane mixtures', *Pure Appl. Chem.* **66**, 553–564 (1994).

9 Commission on Microchemical Techniques and Trace Analysis, 'Separation and preconcentration of trace elements and their physicochemical forms in aqueous media using inert solid membranes', *Pure Appl. Chem.* **66**, 631–640 (1994).

10 Commission on Electroanalytical Chemistry, 'Mercury(II) oxide and silver(I) oxide electrodes in aqueous solutions', *Pure Appl. Chem.* **66**, 641–647 (1994).

11 Commissions on Environmental Analytical Chemistry and Electroanalytical Chemistry, 'Recommendations for electrometric determination of the pH of atmospheric wet deposition (acid rain)', *Pure Appl. Chem.* **66**, 649–658 (1994).

12 Commission on Toxicology, 'Standardized method for estimation of ß-microglobulin, retinol-binding protein and albumin in urine', *Pure Appl. Chem.* **66**, 915–930 (1994).

13 Commission on Polymer Characterization and Properties, 'Properties of ethylene-dimethylaminoethylmethacrylate copolymers as poly(vinyl chloride) resin modifier', *Pure Appl. Chem.* **66**, 1405–1414 (1994).

14 Commission on Colloid and Surface Chemistry including Catalysis, 'Recommendations for characterization of porous solids', *Pure Appl. Chem.* **66**, 1739–1758 (1994).

15 Commission on Microchemical Techniques and Trace Analysis, 'Analytical techniques for trace organic compounds – VI: Application of liquid chromatography-mass spectrometry', *Pure Appl. Chem.* **66**, 1913–30 (1994).

16 Commission on Water Chemistry, 'Structure-activity relationships for biodegradation: A critical review', *Pure Appl. Chem.* **66**, 1931–41 (1994).

17 Commission on Physical Organic Chemistry, 'Compilation and critical evaluation of structure-reactivity parameters and equations – I: Values of and based on ionization of substituted benzoic acids in water at 25 °C', *Pure Appl. Chem.* **66**, 2451–2468 (1994).

18 Commission on General Aspects of Analytical Chemistry, 'Factors important in selection and description of liquid-liquid extraction procedures used in inorganic analytical chemistry', *Pure Appl. Chem.* **66**, 2501–2512 (1994).

19 Commission on Radiochemistry and Nuclear Techniques, 'Determination of very low levels of radioactivity', *Pure Appl. Chem.* **66**, 2537–2586 (1994).

20 *History of IUPAC 1919–87* (published in book form by Blackwell Science, Oxford, 1994).

21 Committee on Publications, *Stereocontrolled Organic Synthesis* (published in book form by Blackwell Science, Oxford, 1994).

22 Committee on Publications, *Chemistry of the Atmosphere: Its Impact on Global Change* (published in book form by Blackwell Science, Oxford, 1994).

23 Commission on Thermodynamics, *Experimental Thermodynamics – Volume IV: Solution Calorimetry* (published in book form by Blackwell Science, Oxford, 1994).

24 Commission on Nomenclature of Organic Chemistry, *A Guide to IUPAC Nomenclature of Organic Compounds* (published in book form by Blackwell Science, Oxford, 1994).

25 Analytical Chemistry Division, *Multilingual Dictionary of Analytical Terms* (published in book form by Blackwell Science, Oxford, 1994).

26 Commission on Solubility Data, Solubility Data Series – Volume 54: *Polycyclic Aromatic Hydrocarbons in Pure and Binary Systems* (published in book form by Oxford University Press, Oxford, 1994).

27 Commission on Solubility Data, Solubility Data Series – Volume 55: *Actinide Nitrates* (published in book form by Oxford University Press, Oxford, 1994).

28 Commission on Solubility Data, Solubility Data Series – Volume 56: *Alcohols with Hydrocarbons* (published in book form by Oxford University Press, Oxford, 1994).

29 Commission on Solubility Data, Solubility Data Series – Volume 57: *Ethene* (published in book form by Oxford University Press, Oxford, 1994).

Twenty-four symposia were sponsored by IUPAC in 1994, namely:

16–20 January 1994. 19th IUPAC Symposium on Chemistry of Natural Products, Karachi, Pakistan. [*Pure Appl. Chem.* **66** (10/11) 1994].

4–9 April 1994. 8th International Conference on High Temperature Materials Chemistry, Vienna, Austria. [*Pure Appl. Chem.* **66** (9) 1994].

4–9 July 1994. 8th IUPAC Congress of Pesticide Chemistry, Washington, DC, USA. (Proceedings published in book form by American Chemical Society, Washington, DC, 1995).

10–14 July 1994. 3rd International Conference on Inorganic Membranes, Worcester, MA, USA. (Proceedings being published by Organizers, anticipated April 1995).

11–15 July 1994. 35th IUPAC International Symposium

on Macromolecules, Akron, Ohio, USA. (Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1995).

17–22 July 1994. 13th IUPAC Conference on Chemical Thermodynamics, Clermont-Ferrand, France. (Rossini and main lectures to be published in *Pure Appl. Chem.,* 1995).

17–22 July 1994. 17th International Carbohydrate Symposium, Ottawa, Canada. (Plenary lectures to be published in *Pure Appl. Chem.,* 1995).

17–22 July 1994. 15th IUPAC Symposium on Photochemistry, Prague, Czech Republic. [*Pure Appl. Chem.,* **67** (1) 1995].

19–22 July 1994. International Conference on Excitonic Processes in Condensed Matter, Darwin, Australia. [*Pure Appl. Chem.,* **67** (3) 1995].

20–21 July 1994. Workshop on Local Air Pollution in Rapidly Developing Countries, Zhen De, nr. Beijing, China. (Technical report to be published in *Pure Appl. Chem.,* 1995).

24–29 July 1994. 30th International Conference on Coordination Chemistry, Kyoto, Japan. [*Pure Appl. Chem.,* **67** (2) 1995].

25–29 July 1994. 35th Microsymposium on Macromolecules and 12th Polymer Networks Group Conference, Prague, Czech Republic. (Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1995).

8–12 August 1994. 13th International Conference on Chemical Education, Puerto Rico. (Proceedings published by organizers, 1994).

22–26 August 1994. 14th International Conference on Raman Spectroscopy, Hong Kong. (Proceedings to be published by John Wiley, 1995).

22–26 August 1994. 6th International Symposium on Solubility Phenomena, Buenos Aires, Argentina. (Main lectures to be published in *Pure Appl. Chem.,* 1995).

28 August – 2 September 1994. 12th International Conference on Physical Organic Chemistry, Padua, Italy. (Main lectures to be published in *Pure Appl. Chem.,* 1995).

29 August – 1 September 1994. 2nd International Symposium on Macrocyclic Ligands for Design of New Materials, Buenos Aires, Argentina. (Main lectures to be published in *Pure Appl. Chem.,* 1995).

6–9 September 1994. International Conference on Liquid Crystal Polymers, Beijing, China. (Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1995).

11–16 September 1994. 6th European Symposium on Thermal Analysis and Calorimetry, Grado, Italy. (Main lectures to be published in *Pure Appl. Chem.,* 1995).

19–22 September 1994. International Conference on Geotoxicology: Mutagens and Clastogens in the Environment, Oxford, UK. (Proceedings to be published by the organizers).

19–23 September 1994. 13th International Symposium on Medicinal Chemistry, Paris, France. (Proceeding to be published in book form by Société Francaise de Chimie Thérapeutique, April 1995).

3–6 October 1994. International Symposium on Molecular Mobility and Order in Polymer Systems, St. Petersburg, Russia. [Proceedings published as Volume 90 (February 1995) of *Macromolecular Symposia* by Hüthig & Wepf Verlag, Basel].

14–16 November 1994. International Symposium on Functional and High Performance Polymers, Taipei, Taiwan, China. (Main lectures to be published in *Pure Appl. Chem.,* 1995).

11–16 December 1994. 10th International Conference on Organic Synthesis, Bangalore, India. (Main lectures to be published in *Pure Appl. Chem.,* 1995).

Fig. 3. The city of Prague, site of the 35th Microsymposium on Macromolecules and 12th Polymer Networks Group Conference

Affiliate Affairs

Information for affiliates

IUPAC publications

Affiliates are entitled to a 25% reduction and in some cases a 40% reduction on the cost of IUPAC publications except the scientific journal *Pure and Applied Chemistry*. A leaflet detailing IUPAC books currently available from Blackwell Scientific Publications has recently been distributed by the publishers to all *CI* readers. Further copies may be obtained from the IUPAC Secretariat.

How to contact commissions

IUPAC affiliates are entitled to communicate directly on scientific matters with the officers of IUPAC commissions. A full list of names and addresses of all commission officers for 1994–95 was published in the November 1993 issue of *CI*.

IUPAC-sponsored conferences

If you are interested in attending a conference please apply directly to the conference organizers for the conference circulars and registration forms. An updated list of names and addresses of the organizers of all future IUPAC sponsored conferences is given in the 'Conference Calendar' published in each issue of *CI*.

Affiliate reduction of conference registration fees

It is a condition of IUPAC sponsorship of a conference that IUPAC affiliates are entitled to a 10% reduction or 'own members' rate on the registration fee for scientific participants. This concession is usually, but not always, announced in the conference circulars and indicated on the registration form.

To receive this reduction an affiliate must declare on the conference registration form that (s)he is an affiliate. Alternatively the affiliate should apply in writing to the conference organizer for this reduction stating that (s)he is an affiliate. Conference organizers may check with the IUPAC Secretariat that applicants for this reduction are currently registered as affiliates.

If an application for this reduction is refused, an affiliate should immediately notify the Affiliate Affairs Secretary and, if possible, forward copies of documentary evidence of this refusal.

Address of IUPAC Secretariat

Please use the following address for all communications directed to the IUPAC Affiliate Affairs Secretary. If your are submitting a letter for publication in *Chemistry International* (*CI*), please indicate that the letter is 'Submitted for publication in *CI*.'

Affiliate Affairs Secretary
IUPAC Secretariat
Bank Court Chambers
2–3 Pound Way
Templars Square
Cowley
Oxford OX4 3YF
UK.
Tel: +44 (1865) 747744
Fax: +44 (1865) 747510
E-mail: iupac@vax.oxford.ac.uk

Ties and scarves

IUPAC ties and scarves may be purchased from the IUPAC Secretariat by applying to the Affiliate Affairs Secretary. The colours for both are *either* maroon *or* navy (dark) blue. The ties cost USD 14.00/GBP 7.00 each and the scarves USD 12.00/GBP 6.00 (including postage and packing).

Please use the form (or a photocopy of it) published on page 24 of the January 1994 issue of *CI*. Alternatively please write to the Affiliate Affairs Secretary with your order stating the colour you require. A cheque made payable to IUPAC for the appropriate amount should be enclosed with your order.

IUPAC poster

Copies of an IUPAC poster are available **free of charge** to affiliates and members of IUPAC's commissions and committees. The poster is printed in maroon and black on a white background and is approximately 42 × 59 cm in size.

IUPAC welcomes any publicity you can give to its activities. If you would like to display one or more copies of the poster in your department or elsewhere please write to the Affiliate Affairs Secretary stating your name and address and how many copies of the poster you wish to receive.

IUPAC Accounts for 1994

Treasurer's comments

Starting with the present financial biennium, expenses for Standing Committees and Divisions are allocated at 70% in the even year and 30% in the odd, rather than allocated wholly in the even year as previously. This means that in a balanced biennial budget there is a substantial surplus in the even year that is balanced by an equal deficit in the odd. This must be borne in mind when reading in the *Summary of Income and Expenses* that there was a surplus of USD148 718 at the year end. Even so, there is cause for satisfaction in that the surplus is some USD27 000 better than budget. Taken together with the surplus of USD22 629 in 1993, this result could be taken to indicate that our current finances are now under control.

At the time of writing, the weakness of the dollar is a matter of concern, but provided that there is an improvement in the value of the dollar within the next month or two, there is hope that the 1995 bottom line will also be better than budget, leading to a balanced biennial account for the first time for several years. This is reassuring when one recalls the forecast made by the Finance Committee at the 1991 Assembly, that if expenses continued to increase at the rate of the previous years and subscriptions were not increased, the deficit in 1994–95 would be about USD500 000.

The positive factors contributing to the 1994 result were: higher than expected, near USD20 000, contributions from Company Associates, a contribution from publications of USD165 000 (USD26 000 above budget), and lower than expected, USD17 500, expenses by the Secretariat. So, for the second year running those guiding our publications affairs have been successful in difficult times.

The principal negative influences were foreign exchange differences of USD19 000, USD17 000 less than the budget figure for income from investments, a not unexpected result for the worst financial markets for several years, and finally, USD10 000 more than budget on contingencies. However, the main component here was the cost of printing the publicity brochures, USD12 000, which had been previously agreed as an exceptional addition to the existing budget.

After a long and detailed examination of the alternatives, it was decided to move our investments and day-to-day banking from the *Union Bank of Switzerland* (*UBS*) to *Merrill Lynch*, New York, and the transfer was made in October. The principal advantages in doing so are seen to be the better performance of *Merrill Lynch*'s investment managers and easier and faster access for both business transactions and discussion of investments. The transfer might have been expected to have a negative effect on the value of the investment portfolio by reason of the charges and losses incurred in having to sell that part of the portfolio held in *UBS* unit trusts (mutual funds) in a depressed market, but this effect was softened by holding the resulting monies in money market funds which, exceptionally, out performed equities and bonds during the latter part of 1994. In what has been described as the worst bond market for 50 years, the loss on our investment portfolio during the year was about 2%, a better result than those of many organizations similar to ours. Our reserves at the end of the year had a book value of USD2365 000, some USD71 000 above the market value and USD287 000 above the 1993 value, but it must be remembered that the new method of allocating funds for Standing Committees and Divisions could lead to a deficit on the Expenses and Income Account in 1995 of USD180 000 (the budget figure) which will be reflected in the value of reserves at that time. The Building Fund was held principally in *UBS* bond funds that had to be sold on transferring the Fund to *Merrill Lynch* and in consequence suffered a substantially greater loss than the main portfolio. At the year end it had a market value of USD288 000 compared with a market value of USD320 000 at the end of 1993.

In conclusion, I would point out that although we appear to have the opportunity of balancing our income and expenses in future, provided that exceptional circumstances do not arise, the monies allocated for our scientific work i.e. to the Divisions, is at about the same real level as it was after the stringent cuts of 1992. If those monies are to be restored to the pre-1992 level we need more income. So, I have again to ask NAOs to do all they can to persuade their funding organizations to pay subscriptions as soon as possible after the beginning of January. There was an improvement at the three month stage in 1994, 22% of total subscriptions compared with 14% in 1993, but at six months the corresponding totals were 31% and 44%. The more essential need though is for new income from persuading the chemical industries to give the Union more support through the Company Associate Scheme.

Publications income and expenses

As auditors of the International Union of Pure and Applied Chemistry we have examined the books of accont and accounts for the year ended 31 December 1994. Our audit was conducted in accordance with auditing standards promulgated by the profession. We confirm that we meet the legal requirements concerning professional qualification and independence.

Based on our examination, we conclude that the books of the account and the accounts are in accordance with Swiss law and requirements of the statutes.

We recommend that the accounts submitted to you be approved.

ZURICH 27 APRIL 1995 **NEUTRA TREUHAND AG**

Comparative balance sheet[1] (expressed in USD)

Liabilities	1994	1993	Assets	1994	1993
Capital Account	2 389 803	2 321 263	Fixed Assets[6]	37 345	42 429
Accounts Payable[2]	23 654	49 327	Cash in Banks[7]	865 287	45 718
Paulo Franzosini Fund	5 659	5 659	Marketable Securities at Cost	1 500 642	2 035 935
Provisions & Subaccounts[3]	190 914	120 727	Building Fund (held in GBP)[8]	288 724	332 959
Prepaid Subscriptions[4]	20 650	1 000	Accounts Receivable[9]	10 029	12 815
Sundry Creditors	10 959	13 787	Sundry Debtor	0	25 910
Capital Gains Realized[5]	–25 493	45 911	Subscriptions, etc., Outstanding[10]	62 837	84 537
Excess of Income over Expenses	148 718	22 629			
	USD 2 764 864	2 580 303		USD 2 764 864	2 580 303

Summary of income and expenses

General Expenses net		–16 211	–116 246
Publications Income net		164 929	148 529
Affiliate Membership Programme Expenses net		0	–9 654
To Capital Account	USD	148 718	22 629

General income and expenses

Income	1994	1993	Expenses	1994	1993
National Subscriptions[11]	599 762	560 310	Office Expenses[15]	312 305	308 952
Company Associate Service Charges[12]	9 350	9 200	Expenses IUPAC Bodies:[16]		
Observer Country Service Charges[13]	650	750	Standing Committees	76 562	46 052
Associated Organization Service Charges[14]	1 650	1 700	Divisions	151 866	85 382
Interest & Dividends Earned	108 207	117 578	General Assembly	7 901	454 537
Debit to Capital Account	16 211	116 246	Bad Debts Write Off[17]	44	30 095
			Bad Debts Provision	–44	–29 000
USD	735 830	805 784	Other Expenses[18]	74 283	83 351
			Foreign Exchange Differences	19 049	–869
			Depreciation	17 792	14 968
			Provisions: Committed Expenses	76 072	–187 684
			USD	735 830	805 784

Publications income and expenses

Income	1994	1993	Expenses	1994	1993
Publications: Blackwell	323 221	323 025	Secretariat (Publications)	170 388	170 439
Publications: Pergamon	732	0	Chem. Intl. to Symposia	557	688
Publications: Other Publishers	16 732	8 297	Miscellaneous Expenses[19]	25 535	31 803
Publications: Secretariat	147	137	Credit to Capital Account	164 929	148 529
BSP Support of Publication Activities	20 000	20 000			
Miscellaneous Income	577	0	USD	361 409	351 459
USD	361 409	351 459			

Affiliate membership programme income and expenses

Income	1994	1993	Expenses	1994	1993
Contributions[20]	75 338	55 336	IUPAC Secretariat	27 360	31 001
Royalties Blackwell	2 309	7 010	*Chem. Intl.* & Leaflets	49 309	53 108
Ties & Scarves	273	135	Miscellaneous Expenses	3 232	3 026
Transfer from General Income & Expenses	1 981	15 000			
Debit to Capital Account	0	9 654	USD	79 901	87 135
USD	79 901	87 135			

Notes to accounts

1. *Accounting policies*

(a) *Basis of Preparation of Financial Statements*

The financial statements are prepared under the historical cost convention.

(b) *Tangible Fixed Assets and Depreciation*

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided on all tangible fixed assets at rates calculated to write off the cost less estimated residual value of each asset on a straight-line basis over its expected useful life as follows:

Fixtures and fittings	over 5 years
Computer hardware	over 5 years

(c) *Leasing Commitments*

Rentals paid under operating leases are charged to the Income and Expenses account on a straight line basis over the period of the lease.

(d) *Foreign Currencies*

Transactions in foreign currencies are recorded at the rate ruling at the date of the transaction. Monetary assets and liabilities are retranslated at the rate of exchange ruling at the balance sheet date. All differences are taken to the income and expenses account, except those incurred in investment transactions, which are taken direct to the balance sheet.

(e) *Investments*

Interest on investment bonds is recognized on a receipts and not an accruals basis.

(f) *Committed Expenses*

The IUPAC Council meets once every two years at the General Assembly to agree budgets for committee operations for the following two years. With effect from 1994, seventy per cent of the budgeted expenses is charged to the income and expenditure account in the first year following the General Assembly and thirty per cent in the General Assembly year.

(g) *Royalty Income*

Royalty income is recognised in the income and expenditure account on a cash received basis.

(h) *Legal Status*

The official headquarters of IUPAC are in Zürich, and the legal domicile of the Union is accepted by the Canton of Zürich as an association under Swiss Law. As such the Union is exempt from any taxation on any net income arising from its activities.

2. *Accounts payable*	**1994**	**1993**
List Oxford	23 654	34 852
List Zürich	–	14 475
	23 654	49 327

3. *Provisions & subaccounts*		
Committed Expenses	76 072	0
Bad Debts	19 950	19 994
CHEMRAWN Conference Loan Fund	15 839	12 781
Neutra Examination	8 000	8 000
History of IUPAC	0	20 000
Purchases from Blackwells/Pergamon	564	1 311
Royal Society Contbn. to Dev. Activs.	19 922	15 845
Kratos Grant	136	136
ICSU Grants	35 184	19 540
Lewis Publishers	5 004	3 004
Organic Synthesis	1 523	1 523
Destruction of Chemical Warfare	6 434	18 593
Oxford University Press		
– Solubility Data Series	2 286	0
	190 914	120 727

4. *Prepaid subscriptions*	**1994**	**1993**
Netherlands NAO 1995	18 100	–
ICC AO 1995	50	–
IOCG AO 1995	50	–
Netherlands CAs 1995	450	–
Egypt CA 1995	450	–
Poland CA 1995	450	–
Russia CA 1995	450	–
Thailand CA 1995	450	–
Bulgaria OC	200	–
IZA AO 1994	–	100
Korea – 2 CAs 1994	–	900
	20 650	1 000

5. *Capital gains realized*		
Capital Gains Realized	–25 493	45 911
Foreign Exchange Differences	0	0
	–25 493	45 911

6. *Fixed assets*		
Fixed Assets	91 586	78 878
Depreciation of Assets over 5 Years	–54 241	–36 449
	37 345	42 429

7. *Cash in banks*		
USD	28 291	26 237
GBP	13 949	14 944
CHF	65	1 215
DEM	0	948
East European Banks (revalued at 91.12.31using relevant exchange rates for national currency to USD; arrangements are in hand to use remaining funds during 1995)		
Bulgaria	0	44
Czechoslovakia	517	517
Hungary	0	545
Poland	0	1 268
Russia	0	0
Money Market Investments	822 465	0
	865 287	45 718

8. *Building fund*

On the recommendation of the IUPAC Council (Minute 7/91, 36th Meeting – Hamburg), part of the Union's assets have been moved into a building fund, to provide for the eventuality that the need for a permanent Secretariat building becomes pressing. Moving the Union's financial business from Union Bank of Switzerland to Merrill Lynch in 1994 entailed selling the UBS unit trusts (mutual funds) which constituted the Building Fund; the consequent loss was USD59 140.

9. *Accounts receivable*		
List Oxford	10 029	11 815
List Zürich	–	1 000
	10 029	12 815

10. *Subscriptions, etc., outstanding*		
National Organizations	62 637	83 837
Observer Country Service Charges	0	50
Company Associates Service Charges	100	650
Associated Organization Service Charges	100	0
	62 837	84 537

	1994	1993
National Organizations (1992)		
Egypt	0	3 800
Greece	0	2 400
		6 200
National Organizations (1993)		
Belgium	0	16 800
Chile	1 800	1 800
China/Beijing	0	200
Egypt	3 800	4 100
Greece	0	2 600
Ireland	0	4 200
Japan	0	29 487
Korea	0	11 000
Turkey	0	3 150
UK	0	4 300
	5 600	77 637
National Organizations (1994)		
Argentina	1 100	–
Belgium	18 200	–
Chile	2 600	–
Egypt	5 500	–
Greece	3 300	–
Israel (CA)	400	–
Japan	23 187	–
Turkey	2 750	–
	57 037	
Service Charges		
Observer Countries (1993)		
Peru	0	50
Service Charges		
Company Associates (1993)		
UK	0	650
Service Charges		
Company Associates (1994)		
Israel	50	–
USA	50	–
Service Charges		
Associated Organizations (1994)		
FECS	50	–
IFCC	50	–
11. *National subscriptions*		
Received	542 725	482 673
Outstanding	57 037	77 637
	599 762	560 310
12. *Company Associate service charges*		
Received	9 250	8 550
Outstanding	100	650
	9 350	9 200
13. *Observer Country service charges*		
Received	650	700
Outstanding	0	50
	650	750

14. *Associated Organization service charges*	1994	1993
Received	1 550	1 700
Outstanding	100	0
	1 650	1 700
15. *Office expenses*		
IUPAC Officers	4 326	3 353
IUPAC Secretariat (Non-pubns.)	272 462	260 020
Audit, Bank Fees, Other Charges	35 517	45 579
	312 305	308 952
16. *Expenses IUPAC bodies*		
Administration Expenses	14 306	35 725
Meetings other than General Assembly	203 022	96 150
Transfer to CHEMRAWN Account	11 100	–441
General Assembly	7 901	454 537
	236 329	585 971
17. *Bad debts write off*		
Bulgaria (AMP)	44	–
Bulgaria (1991)	–	5 100
Bulgaria (1992)	–	2 200
Nigeria (1991)	–	2 400
Nigeria (1992)	–	2 300
Ethiopia (1990)	–	400
Ethiopia (1991)	–	400
Ethiopia (1992)	–	400
Peru (1990)	–	2 100
Peru (1991)	–	2 000
Yugoslavia (1990)	–	3 550
Yugoslavia (1991)	–	4 500
Yugoslavia (1992)	–	4 500
USA CAs (1991)	–	245
	44	30 095
18. *Other expenses*		
Contributions to ICSU	18 857	18 807
Representatives Other Organizations	8 007	8 313
IUPAC Handbook 1989–91	0	15 660
Chem. Intl. for Members	21 195	20 970
Publicity Brochures	12 233	–
Appointment of Information Officer	8 297	–
Miscellaneous Expenses	3 713	4 601
Transfer to Affiliates in Developing Countries	1 981	15 000
	74 283	83 351
19. *Miscellaneous expenses*		
BSP Travel Grant	20 000	28 251
Other	5 535	3 552
	25 535	31 803
20. *AMP contributions*		
In USD	75 338	55 063
From East Europe	0	273
	75 338	55 336

Securities account as at 31 December 1994

Bonds	Currency	Amount	Approx. price %	Approx. value (USD)	Book value at cost (USD)	Profit/(loss) since purchase (potential)
6.5% Toyota	USD	100000	97.31	97312.00	97009.72	302.28
6 3/8% ABB Internat Finance	USD	100000	98.25	98250.00	97634.38	615.62
6.75% Philip Morris Capital Account	USD	150000	97.31	145968.00	148920.00	–2952.00
7% Chubu Electric Power Co. Inc	USD	100000	98.94	98937.00	99019.44	–82.44
4% Sandoz Overs Fin 1991 – 30.9.1998	USD	150000	88.12	132186.98	134562.78	–2375.81
5 7/8% Euro Ciba-Geigy 1993 – 23.3.2000	USD	100000	90.25	90250.00	100260.00	–10010.00
7% Export Dev Corp 1993 – 25.3.1998	USD	150000	67.21	100821.00	120526.37	–19705.37
5.5% General Electric 1993 – 8.4.1998	USD	150000	92.50	138750.00	152280.56	–13530.56
5.75% Osaka Gas 1993 – 26.5.1998	USD	100000	92.69	92687.00	104428.40	–11741.40
5 1/8% Wal-Mart Stores Inc 1993 – 22.10.98	USD	150000	91.06	136593.00	149497.05	–12904.05
US Treasury Bill zero% Feb 16 1995	USD	200000	99.40	198802.00	197960.72	841.28
US Treasury Bill zero% Mar 16 1995	USD	100000	98.92	98916.00	98542.50	373.50
Grand total securities				1429472.98	1500641.92	–71168.95

Conferences

Sixth International Chemistry Conference in Africa
31 July – 4 August 1995
Accra, Ghana

IUPAC SPONSORED

The sixth International Chemistry Conference in Africa has been organized jointly by the Ghana Chemical Society and the Ghana Biochemical Society under the auspices of the Ghana Academy of Arts and Sciences.

In accordance with previous meetings, there will be three types of scientific sessions. There will be a number of Scientific Lectures of an hour duration will be held at the beginning of each afternoon session. Two parallel lectures will take place, catering for two different broad areas, and will deal with detailed scientific research activities taking place in Africa, or of relevance to Africa.

There will be about six parallel sessions for the presentation of scientific papers by participants. Each presentation shall be of 15 minutes' duration, followed by about 5 minutes of discussion. There will also be posters mounted throughout the conference for viewing by participants.

The conference registration fee has been tentatively fixed at USD130, inclusive of lunch and light refreshments during the conference. It is estimated that food will cost between USD10 and USD50 per day depending upon hotel.

All inquiries should be addressed to: The Secretary, 6th ICCA, Chemistry Department, University of Ghana, PO Box 56, Legon, Ghana. Tel.: 233 21 775305, Fax: 233 21 775306 or 776092

Tenth International Conference on Macromolecules, Chromatography of Polymers and Related Substances
18–25 September 1995
Bratislava, Slovakia

IUPAC SPONSORED

The IUPAC International Conference on Chromatography of Polymers and Related Substances will be organized by the Polymer Institute of the Slovak Academy of Sciences and the Slovak Chemical Society, Bratislava, on 18–22 September 1995. The venue for this Tenth Bratislava International Conference on Macromolecules will be the facilities of the Slovak Academy of Science and the Polymer Institute.

The conference will bring together theoreticians as well as experimentalists working in the field of characterization, by chromatographic techniques, of both synthetic and natural polymers, oligomers and related substances. A series of contributions will be devoted to the chromatography of particles and to field-flow fractionation techniques.

The conference will provide an opportunity for meeting scientists from both universities and from industry and testing laboratories. Current results of chromatographic method development and application will be presented including progress in industrial process separation and characterization of complex systems, such as polymer blends and copolymers. The main topics of the conference will be:

- Development of methods, including hyphenated techniques;
- Chromatography of synthetic polymers;
- Chromatography of natural polymers;
- Oligomers and admixtures in polymers.

Bratislava

The registration fee before 1 July 1995 is USD270, after this date it will be USD320. For students and accompanying persons the fee is USD110 and USD130 before and after 1 July 1995, respectively. This registration fee includes lunches. IUPAC Affiliate members are entitled to a 10% discount. A special fee of USD55 is offered to participants from Central and Eastern Europe, this special fee does however, not include meals or some special social events.

Bratislava is the capital of one of the newest European nations. It is situated 65 km from Vienna and 45 km from Vienna International Airport (Schwechat).

Sixth International Symposium on the Harmonization of the Role of Laboratory Quality Assurance in Relation to Total Quality Management (TQM)
4–5 December 1995
Melbourne, Australia

Registration forms are available from: Dr Michael Parkany, ISO Central Secretariat, Case Postale 56, CH-1211 Genève 20, Switzerland, Tel.: (41) 22 749 01 11, Fax: (41) 22 733 34 30, Telex: 41 22 05 iso ch
N.B. Due to limitations of space, registration will be restricted

International Symposium on Chemistry, Biological and Pharmacological Properties of African Medicinal Plants
25–28 February 1996
Victoria Falls, Zimbabwe

This meeting, organized by the Working Group on Plant Chemistry of the International Organization for Chemical Science Development (IOCD), will attempt to bring together scientists from both African and other countries who are involved in the phytochemical investigation of African medicinal plants. An update on different aspects of research concerning the phytochemistry and pharmacology of African plants will be presented.

Participants from both academia and industry are invited to participate. The symposium will feature 12 plenary lectures, six from African speakers and six from non-African speakers. In addition, there will be contributed papers in the form of oral presentations and poster sessions.

For further information, please contact: Prof. K. Hostettmann, Chairman, IOCD Working Group on Plant Chemistry, Institute of Pharmacognosy and Phytochemistry, University of Lausanne, BEP, CH-1015 Lausanne-Dorigny, Switzerland. Tel.: + 41 21 6924561. Fax: + 41 21 6924505

(Bio)Degradable Polymers: Chemical, Biological and Environmental Aspects
15–18 July 1996
Prague, Czech Republic

IUPAC
SPONSORED

The 53rd meeting, 37th microsymposium, of the Prague Meetings on Macromolecules is intended to be an open interdisciplinary forum for both academics and industrial experts, presenting recent ideas and new developments in the field of (bio)degradable polymers. The area selected for discussion will cover the design, synthesis and processing of polymers with intentionally limited lifetimes – (bio)degradable polymers. It is hoped to discuss in detail the mechanisms involved in the degradation processes.

The discussion will focus on the lessons which can be learnt from related fields of science, in particular, biochemistry, biology and environmental science, when considering trends and prospects in the preparation and use of (bio)degradable polymers.

Topics to be discussed include:

- Synthesis, structure and properties of (bio) degradable polymers;
- Mechanisms of (bio)degradation and methods of evaluation of (bio)degrative processes;
- Potentials and prospects of (bio)degradable polymers as utility materials.

There will be a number of invited lectures of 40 minutes' duration and about 15 special communications of 20 minutes' duration. It is hoped to hold a panel discussion on trends and prospects in the preparation and use of (bio)degradable polymer materials.

All sessions of the meeting will be held in the Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám. 2, Praha 6 – Petriny.

Full information and details of registration will be included in the second circular which will be sent out before 11 February 1996. The (approximate) full registration fee will be CHF420, and CHF140 for accompanying persons. This fee includes lunches. Accommodation will be provided in university residences within easy reach of the Institute by public transport. The price of accommodation is not included in the registration fee.

Further details may be obtained from: P. M. M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague, Czech Republic, Tel.: (42) 2360 341, Fax: (42) 2367 981, E-mail: sympo@imc.cas.cz

International Symposium on Sweeteners
14–20 July 1996
Jerusalem, Israel

IUPAC
SPONSORED

The scientific program of this, the first, International Symposium on Sweeteners will discuss all aspects of the chemistry, biochemistry and physiology of sweet materials. It will be an opportunity for the academic, medical and industrial food researchers from all over the world to discuss the future of commercial sweeteners into the next century. Topics to be discussed include:

- natural sweeteners;
- synthetic sweeteners and their synthesis;
- mechanism of gustation;
- health aspects of natural and artificial sweeteners;
- side effects of commercial sweeteners;
- use of sweeteners in food products;
- commercialization of sweeteners;
- sensory characteristics of sweeteners;
- structure-activity relationships amongst sweeteners;
- neurophysiological aspects of sweeteners;
- legislation concerning sweeteners in commercial applications.

For further information, please contact: International Symposium on Sweeteners, PO Box 50006, Tel Aviv 61500, Israel. Tel.: (972) 35140014, Fax: (972) 35175674 and 35140077, E-mail: 100274.2665@CompuServe.COM

Ninth European Conference on Analytical Chemistry. EUROANALYSIS IX.
1–7 September 1996
Bologna, Italy

IUPAC
SPONSORED

The Working Party on Analytical Chemistry of the Federation of European Chemical Societies, the Italian Chemical Society and the Analytical Division of the Italian Chemical Society have organized the ninth meeting of EUROANALYSIS, the European Conference on Analytical Chemistry in the city of Bologna, on 1–7 September 1996.

This triennial conference provides a highly qualified forum for the international scientific community to meet and discuss recent developments in all branches of analytical chemistry. Following the tradition of previous meetings in this series, the ninth meeting will consider all branches of analytical chemistry with emphasis on the 'problem solving' capacity of the discipline.

Sessions on a number of specialized topics are planned, these include:

Education, where the complete scheme of the Euro-curriculum in analytical chemistry will be discussed.
Validation in analytical chemistry.
Reference materials.
Calibration and detectability.

The scientific program will consist of invited lectures and contributed papers, both oral and poster contributions. All contributed papers will be refereed by an international panel. The official language of the conference will be English, there will be no simultaneous translation.

The site of the conference will be *Palazzo della Cultura e dei Congressi*, located in the Exhibition and Fair area of Bologna, a few minutes from the town center. Accommodation will be arranged in a variety of hotels of differing category. A number of low-cost rooms will be available in student rooms.

Bologna is one of the great cities of Renaissance Italy. It boasts one of the oldest universities in the world, certainly the oldest in Europe. The city is a veritable living museum of Renaissance architecture and is full of magnificent libraries, churches and galleries.

Please address all correspondence to:

Prof. Luigia Sabbatini, EUROANALYSIS IX, Dipartimento di Chimica, Universita di Bari, Via Orabona, 4, 70126 Bari, Italy, Tel.: (39) 80 5442020/16/14, Fax: (39) 80 5442026

Bologna.

Conference Calendar

1995

Macrocyclic chemistry

2–7 July
20th International Symposium on Macrocyclic Chemistry.
Jerusalem, Israel.
ISMC, PO Box 50006, Tel Aviv 61500, Israel. Tel.: +972 (3) 5140000.
Fax: +972 (3) 5175674/5140077.

Polymer morphology and electrical properties

5–7 July
International Symposium on Polymer Morphology and Electrical Properties.
Lodz, Poland.
Prof. A. Galeski, Centre of Molecular & Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, 90–363 Lodz, Poland. Tel.: +48 (42) 818952 or 815761. Fax: +48 (42) 847126 or 815483. E-mail: julanski@lodzl.p.lodz.pl.

Analytical chemistry

9–15 July
SAC 95: International Conference on Analytical Chemistry. Hull, UK.
Prof. A. Townshend, School of Chemistry, University of Hull, Hull HU6 7RX, UK. Tel.: +44 (1482) 465027. Fax: +44 (1482) 466410.

Toxicology and clinical chemistry of metals

10–13 July
5th COMTOX Symposium on Toxicology and Clinical Chemistry of Metals.
Vancouver, BC, Canada.
Prof. F. W. Sunderman, Jr., Departments of Laboratory Medicine and Pharmacology, University of Connecticut Medical School, Post Office Box 1292, Farmington, Connecticut 06034–1292, USA. Tel.: +1 (203) 792328. Fax: +1 (203) 6792154.

High swelling gels

10–14 July
36th Microsymposium on Macromolecules - High Swelling Gels.
Prague, Czech Republic.
P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague 6, Czech Republic. Tel.: +42 (2) 360341. Fax: +42 (2) 367981. E-mail: sympo@imc.cas.cz.

Functional dyes

16–21 July
3rd International Symposium on Functional Dyes (Functional Dye '95). Santa Cruz, California, USA.
Dr Kay Kanazawa, IBM Research Division, Almaden Research Center, 650 Harry Road K42/803., San Jose, CA 95120–6099, USA. Fax: +1 (408) 9272213.

Heteroatom chemistry

30 July – 4 August
4th International Conference on Heteroatom Chemistry.
Seoul, Korea.
Prof. Kyongtae Kim, Secretary General, ICHAC-4, Department of Chemistry, Seoul National University, Seoul 151–742, Korea. Tel.: +82 (2) 8806636. Fax: +82 (2) 8748858.

Chemistry in Africa

30 July – 4 August
6th International Chemistry Conference in Africa
Accra, Ghana.
The Secretary, 6th ICCA, Chemistry Department, University of Ghana, PO Box 56, Legon, Ghana. Tel.: +233 (21) 775305. Fax: +233 (21) 775306 or 776092.

Novel aromatic compounds

31 July – 4 August
8th International Symposium on Novel Aromatic Compounds (ISNA-8).
Braunschweig, Germany.
Prof. H. Hopf, Institut für Organische Chemie, Technische Universität, Hagenring 30, D-38106 Braunschweig, Germany. Tel.: +49 (531) 391 5255. Fax: +49 (531) 391 5388

IUPAC General Assembly

4–11 August
38th IUPAC General Assembly.
Guildford, Surrey, UK.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion

Organometallic chemistry directed toward organic synthesis

6–10 August
8th IUPAC Symposium on Organometallic Chemistry directed toward Organic Synthesis (OMCOS-8).
Santa Barbara, California, USA.
Prof. B. H. Lipshutz, Department of Chemistry, University of California, Santa Barbara, California 93106–9510, USA. Tel.: +1 (805) 8933072. Fax: +1 (805) 8937287. E-mail hr03conf@ucsbvm.ucsb.edu.

Heterocyclic chemistry

6–11 August
15th International Congress of Heterocyclic Chemistry.
Taipei, Taiwan, China.
Prof. Chin-Kang Sha, Department of Chemistry, National Tsing Hua University, Hsinchu 300, Taiwan, China. Tel.: +86 (35) 722427. Fax: +86 (35) 725870. E-mail: cksha@chem.nthu.edu.tw.

35th IUPAC Congress

14–19 August
35th IUPAC Congress.
Istanbul, Turkey.
Prof. A. Riza Berkem, Halasgargazi Cad. No. 53, D. 8, 80230 Harbiye, Istanbul, Turkey. Tel.: +90 (212) 2407331. Fax: +90 (212) 2317037.

Plasma chemistry

21–25 August
12th International Symposium on Plasma Chemistry.
Minnesota, Minneapolis, USA.
ISPC-12, c/o Catherine Ploetz, 218 Nolte Center, University of Minnesota, 315 Pillsbury Drive SE, Minneapolis, MN 55455, USA. Tel.: +1 (612) 6262259. Fax: +1 (612) 6261632. E-mail: ispc12@pdcs.cee.umn.edu

Spectroscopy

27 August – 1 September
29th Colloguium Spectroscopicum Internationale. Leipzig, Germany.
CSI XXIX Secretariat, Gesellschaft Deutscher Chemiker, Abt. Tagungen, Postfach 90 04 40, D-60444 Frankfurt am Main, Germany. Tel.: +49 (69) 7917358. Fax: +49 (69) 7917475.

Liquid and amorphous metals

27 August – 1 September
9th International Conference on Liquid and Amorphous Metals.
Chicago, USA.
Drs Saboungi and Price, Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA. Tel.: +1 (708) 252 4341 (M.-L. Saboungi), +1 (708) 252 5475 (D.L.Price) Fax: +1 (708) 252 7777.

Industry – education initiatives in chemistry

28 August – 2 September
International Symposium on Industry – Education Initiatives in Chemistry.
York, UK.
Dr J. F. Gibson, The Royal Society of Chemistry, Burlington House, Piccadilly, London WIV OBN, UK. Tel.: +44 (171) 4378656. Fax +44 (171) 7341227.

Solution chemistry

29 August – 2 September
24th International Conference on Solution Chemistry.
Lisbon, Portugal.
Prof. C. A. N. Viana, Instituto Bento da Rocha Cabral, F.C.U.L., Calçada Bento da Rocha Cabral, 1200 Lisboa, Portugal. Tel.: +351 (1) 3859628/608823. Fax: +351 (1) 7977837.

Medicinal chemistry

3–8 September
AFMC International Medicinal Chemistry Symposium (AIMECS 95). Tokyo, Japan.
Prof. S. Ikegami, Secretary General, AIMECS 95, c/o Faculty of Pharmaceutical Sciences, Teikyo University, Sagamiko, Kanagawa 199–01, Japan. Tel.: +81 (426) 850161. Fax: +81 (426) 851870.

Ionic polymerization

4–8 September
1st International Symposium on Ionic Polymerization.
Istanbul, Turkey.
IUPAC International Symposium on Ionic Polymerization, c/o Prof. Y. Yagci, Istanbul Technical University, Faculty of Science, Department of Chemistry, Maslak 80626, Istanbul, Turkey. Tel.: +90 (212) 285 32 41. Fax: +90 (212) 285 63 86. E-mail: Feyusuf@TRITU

Applications of the mössbauer effect

10–16 September
International Conference on the Applications of the Mössbauer Effect (ICAME-95).
Rimini, Italy.
Prof. I. Ortalli, ICAME-95, University of Parma, Istituto di Scienze Fisiche, Via M. D'Azeglio 85, I-43100 Parma, Italy. Tel.: +39 (521) 902231. Fax: +39 (521) 236508. E-mail: ICAME95@ipruniv.cce.unipr.it

Bioorganic chemistry

17–23 September
3rd International Symposium on Bioorganic Chemistry.
Dagomys, Sochi region of Black Sea Coast, Russia.
Dr V. V. Demin, Shemyakin - Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Ul. Miklukho-Maklaya, 16/10, 117871 Moscow V-437, Russia. Tel.: +7 (095) 3351511, 330–6338, 3302800. Fax: +7 (095) 3107007.

Chromatography of polymers

18–22 September.
International Symposium on Chromatography of Polymers and Related Substances.
Bratislava, Slovakia.
Dr D. Berek, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, Sk-842 36 Bratislava, Slovakia. Tel.: +42 (7) 3782306. Fax: +42 (7) 375923.

Assessment carcinogenic risk

17–20 October
International Symposium on the Assessment of Respiratory Carcinogenic Risk from Occupational Exposure to Inorganic Substances. Luxembourg.
Dr J. H. Duffus, Director, The Edinburgh Centre for Toxicology, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS, Scotland. Tel.: +44 (131) 4513456. Fax: +44 (131) 4513017.

Environmental catalysis

25–27 October
2nd International Forum on Environmental Catalysis. Tokyo, Japan.
Prof. Eiichi Kikuchi, General Secretary IFEC'95, Department of Applied Chemistry, School of Science and Engineering, Waseda University, 3–4-1, Okubo Shinjuku-ku, Tokyo 169, Japan. Tel.: +81 (3) 32005349. Fax: +81 (3) 32005349. E-mail: ekikuchi@cfi.waseda.ac.jp.

Soil chemistry and ecosystem health

28 October
Workshop on Soil Chemistry and Ecosystem Health. St. Louis, MO, USA.
Prof. P. M. Huang, Department of Soil Science, University of Saskatchewan, Saskatoon, Saskatchewan S7N OWO, Canada. Tel.: +1 (306) 9666823. Fax: +1 (306) 9666881.

Automation and new technology in clinical laboratory

2–4 November
6th International Congress on Automation and New Technology in Clinical Laboratory. Sitges, Barcelona, Spain.
ANT/CCL/SEQC/95, Llançà 51, 08015 Barcelona, Spain. Tel.: +34 (3) 2269827. Fax: +34 (3) 2266969.

Macromolecule–metal complexes

3–6 November
6th International Symposium on Macromolecule–Metal Complexes (MMC-VI). Guangzhou, China
Prof. Ying-Yan Jiang, Institute of Chemistry, Academia Sinica, Zhongguancun, Beijing 100080, China.

1996

Phenothiazines and related psychotropic compounds

26–29 February
8th International Conference on Phenothiazines and Structurally Related Psychotropic Compounds. Jaipur, India.
Dr R. R. Gupta, Department of Chemistry, University of Rajasthan, Jaipur-302 004, India.

Free-radical polymerization

26–31 May
2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism. Santa Margherita Ligure, Genoa, Italy.
Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy. Tel.: +39 (79) 229556. Fax: +39 (79) 229559

Mycotoxins and phycotoxins

27–31 May
9th International Symposiums on Mycotoxins and Phycotoxins. Rome, Italy.
Dr Marina Miraglia, Instituto Superiore Sanità, Food Department, Viale Regina Elena, 299, I-00161 Rome, Italy. Tel.: +39 (6) 4990, ext. 377. Fax +39 (6) 4451767.

Organic synthesis

30 June – 4 July
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Conference Secretariat ICOS - 11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (80) 234471. Fax: +31 (80) 601159.

Catalysis

30 June – 5 July
11th International Congress on Catalysis. Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520–8286, USA. Tel.: +1 (203) 432 4378. Fax: +1 (203) 432 4387.

Chemical education

14–19 July
14th International Conference on Chemical Education – Chemistry: Expanding The Boundaries. Brisbane, Australia.
Dr W. Beasley, Graduate School of Education, The University of QAueensland, Brisbane, Queensland 4072, Australia.

How to apply for IUPAC sponsorship

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International Union of Pure and Applied Chemistry (IUPAC)

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.
Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

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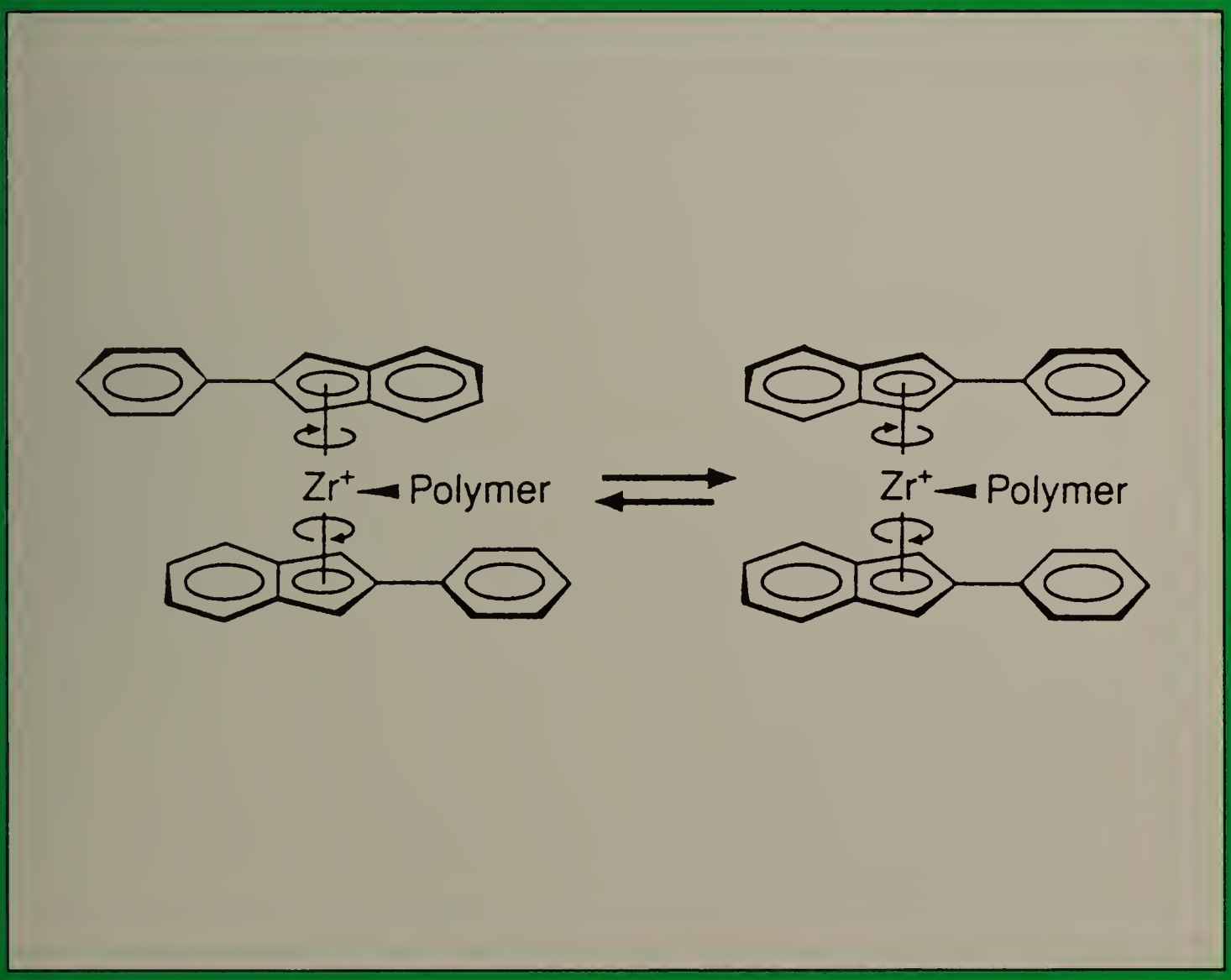

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Front cover: Stereoblock polymer formation.

International Union of Pure and Applied Chemistry

Ethics in modern science – a framework for discussion

Joshua Jortner

Professor Joshua Jortner is President of the Israel Academy of Sciences and Humanities, he is a physical chemist of international renown, well known for his work on intramolecular and condensed phase dynamics. He is a member of the Executive Committee and the Bureau of IUPAC, and of the Subcommittee on Ethics in Science.

Professor Jortner is a physical chemist of international renown.

Introduction

Science is unique amongst human endeavours in that its entire edifice, and continued advance, rests on the honesty and the personal integrity of its practitioners, scientists. It is a collective effort in which each individual scientist can, hopefully, depend on the truthfulness of other scientists.

Ethical guidelines of conduct for scientists have existed for as long as the scientific enterprise. Due to direct public exposure, this is particularly the case in the bio-medical field. In the past, these guidelines were largely unwritten, but the rapid growth of science, and the increase in the number of scientists this century has perhaps created a need for renewed discussion and more explicit formulation of the problem of ethical standards in science.

Moreover, as Philip H. Abelson aptly notes in an editorial (*Science*, 30 October 1992) 'a confluence of factors has led to unusual uncertainty concerning support of scientific research. These factors include the end of the Cold War, global economic competition, federal and state budget deficits, loss of faith in basic research as a key to prosperity, and diminished public esteem for academic research. The latter is due to publicity about fraud in science and a few instances of faulty bookkeeping of grant overhead charges.' The scientific community as a whole should do its utmost to restore the public's confidence in science. It is likely that a clear statement of the ethical principles to which all scientists must conform would greatly contribute to the improvement of the public's trust in the scientific enterprise.

The US National Academy of Science was among the first of a number of nongovernmental scientific bodies to recognize the need for a renewed discussion on the ethical guidelines for scientific research, with the aim of making them more explicit. In a report (*Responsible Science: Ensuring the Integrity of the Research Process*, 1992), the president of the US National Academy of Sciences clearly formulated these needs: 'the broader scientific community knows that ensuring the integrity of the research process is fundamental to the success of science. Scientists must also recognize that it is requisite to the continuing support of science with public funds'.

There are two important aspects to the work of natural scientists, the one internal, relating to the development of the intellectual and conceptual framework of science, and the other external, relating to the interrelation between social and scientific values and activities. Scientists have always had a social and moral responsibility, extending both to their role in shaping the intrinsic values of science and the implications of their research in the broader social context.

These ethical issues in science can be categorized as:

(i) internal – pertaining to the norms of conduct of scientific research and the publication of its results;

(ii) external – pertaining to:

(a) the consequences of scientific activity, and of scientific discoveries on, for example, individuals, groups, societies, indeed, mankind at large, i.e. the effect of science on society;

(b) the socio-cultural environment within which scientific research is conducted. The scientific endeavour can only be undertaken with regard to its place in society. Scientists completely divorced from society would not be a good idea.

Internal ethical issues of science

A close examination of how the scientific community operates, shows that there are many reasons why ethical guidelines have been acknowledged as essential within the scientific community. These include:

1 Fostering integrity in a politically and socially changing research environment. Even in an advanced nation, governments can move suddenly to impose changes on the national science policy support system, but it would be hoped that this would not affect the way science is undertaken.

2 Imposing an internal self-regulatory system in science. It would be hoped that scientists could regulate their own affairs without the need for intervention by nonscientists.
3 Enhancing the contributions of the intrinsic values of science to modern society.
4 Inspiring public confidence in science. This is of paramount importance as too often today the general public when they think of chemistry or physics think of toxic waste dumps and cancer-causing chemicals and radiation. The public does not think of the many advances that science has given to mankind, for example, the continuing lengthening of life expectancy.
5 Enhancement of moral and material public-support for science. Anything which will increase the scientific literacy of the general public is to be welcomed.
6 Providing leadership to the younger generation of scientists. The scientific enterprise must continue, and it is hoped that the best values of one generation will be passed onto the next generation by teaching and example.

Norms of scientific activity and their violation

A number of scholars have attempted to define the norms of scientific activity. Robert Merton ('The normative structure of science' in, N. Storer (ed.), *The Sociology of Science: Theoretical and Empirical Investigations*, Chicago University Press, 1973) defined the norms of scientific activity as follows:

- universalism, i.e. adhering to accepted intellectual criteria;
- disinterestedness, i.e. the extension of scientific knowledge by unselfish engagement, as represented by most basic research;
- scepticism, i.e. empirical and logical tests of claims and results;
- communalism, i.e. openness and information sharing, which constitutes a true internationalism.

M. Mohr ('The Ethics of Science', in *International Science Reviews* **4**, 45 (1979)) presented a list of normative rules: 'Be honest; never manipulate data; be precise; be fair with regard to priority; be without bias with regard to data and ideas of your rival; do not make compromises in trying to solve a problem.'

Violation of such norms of scientific activity is sometimes loosely called 'fraud'. However, in both everyday and legal language, fraud is defined as criminal deception, or as the use of false information with intent to benefit the deceiver. When a scientist knowingly uses false data to try to secure a position, to obtain public or private research funds or to benefit personally in other ways, that is fraud. For most types of violation, however, 'misconduct' is a sufficiently strong term. Although cases of misconduct or actual fraud in science are rare (there were fewer than 100 confirmed cases of misconduct in science in the United States during 1980–90), they should be taken seriously by the scientific community.

The precise definition of misconduct in science remains difficult and controversial. A case in point is the aforementioned report on 'Responsible Science' issued by a committee of the US National Academy of Sciences. The committee, chaired by E. E. David, defined scientific misconduct as 'fabrication or plagiarism in proposing, performing, or reporting research.' However, Howard Schachman and Keith Yamamoto criticized the report in a minority statement for 'failing to convey the overriding importance of intellectual freedom.' The US National Science Foundation contended that while the David committee report had adopted part of a definition currently in force at the National Science Foundation and the National Institute of Health, it lacked an additional clause 'or other serious deviations from accepted research practices.' On the positive side, the David Committee concluded that 'the existing self-regulatory system in science is sound.'

Rules of publication

Publication of scientific discoveries has always been the primary means of relaying the progress of science to the contemporary scientific community, and to future generations of society. Integrity and quality control in this area are vital both to the advancement of science and to maintaining public confidence. The following ethical ground rules have gained, albeit implicitly, almost universal acceptance:
(i) accurate scientific reporting must adhere to the norms of objectivity, honesty, precision and recognition of priority;
(ii) the results of scientific research should be published in scientific journals edited by scientists with appropriate expertise, and using external referees who, it is hoped will guarantee quality control of manuscripts by means of peer review;
(iii) the referees, chosen by the editor and usually anonymous, must adhere to strict criteria of integrity (however, this is not really subject to external regulation);
(iv) temporary embargo on public disclosure: the public announcement of scientific results should be with held until they are accepted for publication in a scientific journal which fulfils criterion (ii).

These guidelines should be self-evident, but they are not always followed. In particular, occasional deviations from the norm of disinterestedness have led to violations. A case in point appeared in *Science* (30 October 1992: Rustum Roy: 'PR is a Better System than Peer Review') reporting a senior scientist's opinion that 'peer review is a terrible process: too slow and too leaky, allowing peer reviewers to gain research advantages unfairly'.

The public's declining trust of the objectivity of scientific publications is indicated in an article published in *Newsweek* (September 28, 1992; p. 50) entitled 'Is Science Censored? Ideology May Influence What Gets Published'. The article's author states that 'To be sure, science is not routinely censored ... If science loses its reputation for probity, its conclusions will carry no more weight than any interest group's'.

External ethical issues in science

(a) The consequences of scientific activity (science on society)

Public scrutiny tends to focus on external issues, such as the implications of scientific activity in the world of military, economic environmental and biomedical affairs. However, responsibility for the social and global implications of scientific research extends both to individual scientist and to the national and international scientific communities.

The use (or abuse) of science for destructive purposes is as old as warfare. In modern times, however, the development of weapons of mass destruction has made this a matter of deepening concern. Attempts at control have been undertaken by individual scientists, groups of scientists (such as the Pugwash Committee) and Learned Societies. The Pugwash Committee is probably the most successful forum for discussions on limiting the results of the misuse of science. These conferences have been running for many years and seek, even though they shun too much publicity, to increase awareness amongst scientists, and scientific advisers, of the possible consequences of maintaining stockpiles of nuclear weapons.

Scientific and technological advances in such areas as nuclear energy, genetic engineering and transplant techniques have raised profound questions regarding their appropriate utilization. Addressing these issues will require a collective effort on the part of the entire scientific community, transcending the boundaries of the various disciplines. An example of this kind of effort is the intensive activity currently taking place in the realm of bioethics, as manifested in the European convention drafted in Madrid (*Nature* **356**, 368 (1992)), the bill passed by the French Senate, and the London Council on Bioethics (*Nature* **356**, 368 (1992)).

(b) The environment within which science is conducted (the scientist in society)

Universal ethical codes of conduct, enshrined in human thought since ancient times, have relevance to the conduct of scientific research and the environment within which it is conducted. These include, for example, the freedom of cultural exchange and the sanctity of human life. A notable example in this area is the principle of the free mobility of scientists, which constitutes a basic condition for the freedom of scientific creativity. The International Council of Scientific Unions (ICSU), as well as many Academies of Sciences have integrated this principle into their ethical codes of conduct and taken action on them.

When a serious breach of the ethics of society occurs, this can have profound consequences for the activity of professionally trained scientists. The history of the twentieth century contains dark chapters of crimes perpetrated in the name of science by scientists. This misuse or perversion of science does not fall into any comprehensive category of scientific research. Such activities are not merely a misuse of science; they are a breach of the ethical code of modern society and have rightly been termed crimes against humanity.

Recommendation regarding the activities of IUPAC in the area of ethics in chemical science

Jan Hult (Chalmers University of Technology, Gothenburg) proposed the following useful distinction between several levels of ethics.

1 *Laws of scientific research*. These are enforced in many countries; examples are regulations on the use of drugs or on experimentation with animals.

2 *Ethical rules*. These are advanced by public organizations responsible for financial support of basic research, such as councils and science foundations. Their responsibility helps to ensure the freedom of research from excessive government intervention.

3 *Ethical guidelines*. These are less formal, personal, institutional, national and international rules which pertain to the application of research results.

4 *Ethical codes of conduct*. These are formulated by learned societies, such as Academies of Science, to ensure the preservation of international norms and standards of scientific conduct.

When considering what are necessary ethics for the conduct of research, a clear distinction should be made between different levels of scientific ethics – from the more diffuse and abstract recommendations to the more definitive and concrete norms of action.

IUPAC, for example, constitutes the international professional body of chemists, and, as such, the sole international authoritative and objective institution of chemical science. Like other governing bodies of individual disciplines, IUPAC has a responsibility for issues falling within its purview.

In view of IUPAC's scientific and human responsibility to the younger generation, and the significance of 'public relations' both within and beyond the scientific community – it should undertake to formulate the explicit ethical guidelines and codes of conduct pertaining to chemical research and its implications. These should relate to:

(a) internal issues pertaining to misconduct in research (e.g. with respect to intellectual property), publication (e.g. authorship, conflict of interest), and to the establishment of international standards (e.g. data selection, research design and safety);
(b) external issues pertaining to the implications of chemical research, within the context of the universal ethical values accepted by the scientific community as a whole (e.g. regarding the development of chemical weapons, or environmental problems).

This article constitutes an attempt to formulate a code of ethics for scientists. IUPAC is conscious of its responsibilities in this difficult area of scientific ethics. Likewise, various national chemical societies have formulated their own ideas on this subject, for example, the National Academy of Science in the US has published, ***On Being a Scientist: Responsible Conduct in Research****, 2nd Ed., 1995, and the American Chemical Society regularly publishes in its journals,* ***Ethical Guidelines to Publication of Chemical Research****. Comments on the contents of this article are welcomed, and should be sent to the editor at the Oxford Secretariat.*

The Scientist and Ethics: Cautionary Tales

A recent report of US Congressional activities has highlighted a growing problem for experimental scientists, that of their perceived integrity. A member of the recently created US **Commission on Research Integrity** suggested that a confidential study be carried out to check the correspondence between raw data and those data appearing in published papers, in order to discover the extent of scientific fraud or scientific misconduct – the creation of a 'data police.'

The idea of such a cross-check was first mooted in 1989 by Desmond Rennie, a professor of medicine at the University of California and a commission member. At a recent meeting of the commission in Washington, DC, Kristina Gunsalus, vice-chancellor for research at the University of Illinois at Urbana-Champaign and another member of the commission admitted that Rennie's suggestion had met with howls of protest.

However, this idea of checking the veracity of published data, ensuring that scientists are not over-indulging in creative fiction, has gained support from other members of the commission. For example, the chairman, Kenneth Ryan hoped that 'If everyone was told when they submitted a paper that their data might be requested confidentially, I would hope that it would be obvious that they would agree.'

Gunsalus claims that a study of the integrity of published data should not be thought of as an assault on scientists. However, she points out that there is no hard data to support the scientific establishments oft-quoted assertion that there is little or no scientific fraud.

This lamentable state of affairs has apparently arisen from the frustration of the US Congressional Commission by the way accusations of scientific misconduct against the National Institutes of Health (NIH) have been handled, or rather not handled, by the NIH. In particular, it is deemed that the NIH's Office of Research Integrity (ORI), which investigates claims of misconduct, has not been working as Congress had hoped.

Ryan's panel will investigate the competence of the ORI and advise on definitions of misconduct, and on how allegations of misconduct should be treated and the scientists who, for whatever reason, have made the allegations against their colleagues, whistleblowers in the language of the investigating authorities, should be protected.

As a case example, the ORI has published its long-awaited report on the misconduct of Dr Theresa Imanishi-Kari, coauthor with the Nobel laureate David Baltimore of a controversial immunology paper. The ORI found Imanishi-Kari guilty of 19 charges of scientific misconduct. The specific conclusions of the report are that Imanishi-Kari fabricated and falsified critical parts of her published results, and that she compounded this by denying the misconduct and fabrication. The report also concludes that she 'further compounded the fabrications and falsifications by referencing or reporting them in grant applications submitted to the NIH'.

This controversy began in 1986 when Dr Margot O'Toole, a Post Doc in Imanishi-Kari's laboratory noticed that the data in a laboratory notebook did not support those that had been published. She claims that she was also put under pressure to report her own data in a misleading manner. The original data was subpoenaed by a congressional subcommittee who opened their own investigation.

O'Toole was for a long time cold-shouldered in academic circles, but does now have a position.

This extraordinary case does not end here. The final scenes in this nine-year drama are currently being enacted in a court room in Washington, DC, with federal government lawyers presenting their case against Imanishi-Kari.

Imanishi-Kari asserts she is innocent of any wrongdoing. She asked for this appeal hearing after the ORI had published its report. If the ORI decision is upheld by this appeal board, Imanishi-Kari will be barred from receiving federal grants or contract money for 10 years. The proceedings, which resemble a trial, is conducted by a three-member appeals board of the Department of Health and Human Services, two lawyers and an immunologist.

'The evidence will show that this is one of the most egregious cases of scientific misconduct ever encoun-

tered by ORI', said the ORI lawyer in his opening statement (*C&E News* June 19, 1995). Not only did Imanishi-Kari misrepresent her research in the publication, he said, but 'she then deliberately set out to fabricate and falsify additional data to support the claim in the paper.' To prove their assertion that the data in Imanishi-Kari's laboratory notebooks was tampered with after the date at which the experiments were purportedly done, the ORI have enlisted the assistance of agencies of the federal government to undertake a forensic analysis.

Testimony for, and against, Imanishi-Kari has been presented by eminent scientists. Nobel laureate Walter Gilbert of Harvard University reiterated his opinion that key data in the original paper were fraudulent. While another Nobel laureate, David Baltimore, a coauthor of the original paper (he and all other coauthors of the original paper – except Imanishi-Kari – retracted the paper in 1991), testified that the results given in the paper had stood the test of time.

The Commission on Research Integrity has said that, '*misconduct is defined as fabrication, falsification, plagiarism and other practises that seriously deviate from those that are commonly accepted within the scientific community for proposing, conducting, or reporting research. It does not include honest error or honest differences in interpretations or judgements of data.*' The third category which is particularly pernicious and contentious as it covers issues such as authorship, the degree of supervision of, presumably, a junior scientist by a senior scientist and various problems which arise within the peer review process of publishing and grant applications.

As publishing is to a certain extent about human vanity, rather than a purely altruistic desire to disseminate the results of one's research, passions can and do run high. This is a particular problem for the scientific world where interpersonal skills and the ability to communicate effectively are not as highly prized as they should be.

The congressional commission is seeking to divide misconduct into two classes of misbehaviour, one which can be regulated by the scientific establishment, who would be expected to set up criteria to be used in regulating standards of behaviour across disciplines and institutions, and the other class of misbehaviour, the more serious, which will require regulation by federal authorities.

However, some scientists are unhappy about, what they consider, to be loose or ambiguous terms in the above definition of misconduct. For example, some scientists fear that the 'serious deviations' clause could be used to harass unconventional researchers. Many are saying that the definition of misconduct should be limited to fabrication, falsification and plagiarism. However, all agree that what is required is a form of words which clearly shows that misconduct is wrong. The following definition has been proposed by some members of the Commission. '*Research misconduct is behaviour that corrupts the scientific record or compromises the objectivity of science in federally funded programs. Research misconduct is defined as intentional or reckless conduct by an individual, the result of which is to seriously misrepresent, interfere with, or misappropriate the content of federally funded research activities, whether in proposing, reviewing, conducting or reporting such activities. Research misconduct does not include honest error or honest differences in interpretations or judgements of data*' (*C&E News* July 3, 1995). It is also proposed that universities, which receive federal funding, be required to give their graduate students some training in ethical issues.

This demand by our elected representatives that they regulate an activity in which the vast majority of them have little or no interest, let alone the necessary training to comprehend, tells us much about the lowly status of the scientist in society. The politicians deem that the scientific establishment cannot run its own affairs and that they know best. This is an interesting proposition, few politicians today are widely respected by the general public. Indeed, many politicians, even those democratically elected, are reviled, being considered avaricious and self-serving.

It is undoubtedly true that some scientists fabricate data and steal their colleagues results. However, we have created a society obsessed by success, winning, or being first, is everything. In science, the pithy little phrase 'publish or perish' has become a litany for many. Unfortunately, in today's society, scientists are judged by grant awarding bodies and panels for promotion on their publication record which needs to be as long as possible.

Public exposure of those who give in to the temptation, and indulge in misconduct, does nothing but bring all scientists into disrepute – they appear to have no sense of responsibility. This is a grave accusation in a world increasingly shaped by science and technology, where scientific and technological literacy are not widely found among ordinary people, who will therefore be forced to turn to the scientist to help them come to terms with our changing society. The scientist is needed in our society, he should not become distracted.

To escape this unwanted and unnecessary public attention, scientists must put their own house in order. If they are seen to behave in an irresponsible way with public money, which is becoming increasingly scarce for research, and to abuse the fragile and easily manipulated methods of gaining promotion and advancement, then they will be forced, against their will, to reform themselves by interfering politicians who know nothing about science. This embarrassing situation will then further erode public confidence in science and the scientist.

(Jeffrey H. Williams)

The Chemical Heritage Foundation

The Chemical Heritage Foundation represents the chemical community putting its past to work to ensure our future.

Introduction: origins

Researchers, industrialists, and entrepreneurs in the chemical sciences have revolutionized our understanding of the world around us, improved our control of disease, and increased the longevity and quality of our lives. They are the true, unsung heroes of the twentieth century. There is hardly a breakthrough in nutrition, modern medicine, biotechnology, electronics, computers, home furnishings, automobiles, or commercial or space travel that does not involve chemistry or a chemical process. If these achievements, and the vast stores of information which represent the heritage of the chemical sciences and industries, are to be properly researched, recorded, and disseminated, the worldwide chemical community needs to nurture and maintain its own center of accurate, reliable, objective information to which the media, legislators, science writers, scholars, historians, school teachers, and chemical scientists can refer, the Chemical Heritage Foundation meets this need.

Far too often, either through lack of knowledge or media-fed sensationalism, the public associates the chemical sciences and their industries primarily with cancer, pollution, and environmental abuse. Through its growing array of information resources and academic and public education services, the Chemical Heritage Foundation is well positioned to offer a more balanced perspective, and to highlight the achievements which have moved our civilization forward.

It was an American Chemical Society initiative, in response to the urgent need to document, preserve, and make known our extraordinary heritage of chemical achievement, that prompted the creation in 1982 of the *Center for the History of Chemistry* at the University of Pennsylvania. The Center's success led to the incorporation in 1987 by the American Chemical Society and the American Institute of Chemical Engineers of what is now the Chemical Heritage Foundation. The Foundation is a public charity under the applicable provisions of the Internal Revenue Code, and all donations to it are tax-deductible.

Mission and operating structure

The Chemical Heritage Foundation seeks to advance the heritage of the chemical sciences and the chemical process industries. To do so, the Chemical Heritage Foundation supports the discovery and dissemination of historical resources; encourages research, scholarship, and popular writing on issues of public interest and debate; publishes resource guides and historical materials; conducts oral histories; creates traveling exhibits; and serves as the central resource for individuals seeking to enhance public understanding of the chemical sciences and the chemical process industries.

The Chemical Heritage Foundation fulfills its responsibilities through the synergism of the public education and academic programs of its *Arnold and Mabel Beckman Center for the History of Chemistry* and the development of resource collections by its *Donald F. and Mildred Topp Othmer Library of Chemical History*, which is fast becoming the premier information repository, media resource center, and research facility for the chemical sciences. The Beckman Center and the Othmer Library are interrelated and mutually supporting resources. The quality and breadth of the Beckman Center's public education and academic research initiatives depend heavily and directly on the Center's access to information resources. At the same time, without the Beckman Center's activities, the substantial historical resources which comprise the Othmer Library would not be utilized to their full potential. The Chemical Heritage Foundation requires a permanent home with the requisite size and historical appeal to properly house the heritage of the chemical sciences and the chemical process industries and where allied efforts such as a museum could be undertaken.

In pursuing its mission and conducting its activities, the Foundation has established fundamental goals, which include: creating a more scientifically literate citizenry, increasing the flow of our most able students into the chemical sciences and industries, and instilling in chemical scientists and practitioners a greater pride in their contributions to society.

The careful nurturing of the symbiosis between the Beckman Center and its sister Othmer Library is essential to the achievement of these fundamental goals.

Governance

The Foundation is under the oversight of a Board of Directors comprised of representatives from its founding members (American Chemical Society and the American Institute of Chemical Engineers), eleven affiliated chemical organizations (The Chemists' Club, Inc.; The Electrochemical Society, Inc.; American Society for Mass Spectrometry; American Association of

Textile Chemists and Colorists; *Société de Chimie Industrielle;* The American Association for Clinical Chemistry, Inc.; Alpha Chi Sigma; The American Institute of Chemists, Inc.; Federation of Societies for Coating Technology; American Oil Chemists' Society; and Chemical Manufacturers Association), and six members at-large. Charles C. Price, a renowned polymer chemist and past President of the American Chemical Society was its Founding Chairman. Today, the Chemical Heritage Foundation is chaired by Sheldon E. Isakoff, a distinguished chemical engineer and former President of American Institute of Chemical Engineers. The Board's actions are guided by input from the Executive, Finance, Nominations, Personnel, Program, and Development Committees.

The Development Committee is headed by John C. Haas, former Chairman of the Board of the Rohm and Haas Company. An Advisory Board of distinguished academics and leaders of industry, including Alan R. Hirsig (ARCO Chemical), Robert A. Ingram (Glaxo), Robert D. Kennedy (Union Carbide), Frank P. Popoff (Dow Chemical), and J. Lawrence Wilson (Rohm and Haas), provides both financial and technical support. Among the Foundation's Board of Directors and Advisory Board members, three (Herbert C. Brown, Roald Hoffmann, and Glenn T. Seaborg) are Nobel Prize winners. The Foundation also draws on the support and expert advice of a widely representative Council of Friends chaired by Priestley Medal winner Howard E. Simmons, Jr. The Executive Director of the Foundation is Dr Arnold Thackray, a former industrial chemist with a research degree in history from Cambridge. Dr Thackray holds the Joseph Priestley Professorship at the University of Pennsylvania and is well known as the author and editor of numerous books and articles on the history of science and technology.

As a public charity, the Foundation derives its operating income primarily from annual gifts by corporations, foundations, professional organizations, and individuals, as well as from interest on assets of about $5 million. Three generous benefactors, inventor Donald F. Othmer, who is most widely known as editor of the Kirk–Othmer *Encyclopedia of Chemical Technology*; Arnold O. Beckman, of pH meter and spectrophotometer fame; and the late chemist/historian and Chairman of the Dexter Chemical Corporation, Sidney M. Edelstein, have supported much of the Foundation's work to date.

Public education and academic programs/ Beckman Center for the History of Chemistry

Public education programs are the avenue through which the Chemical Heritage Foundation can affect, in a positive way, public attitudes towards the chemical sciences and industries, help all citizens become more scientifically discerning, and influence policies which have a direct impact on our social welfare. To that end, the Chemical Heritage Foundation, through its *Arnold and Mabel Beckman Center*:

- Develops traveling exhibits such as
  - *Polymers and People*;
  - *R. B. Woodward and the Art of Organic Synthesis, Scaling Up*;
  - *Structures of Life*;

  which highlight the contributions of chemical scientists and the chemical process industries to society. These exhibits, which are accompanied by illustrated booklets, tour world-wide to schools, museums, science centers, and professional meetings;
- Conducts summer workshops with high school chemistry teachers. The objective of the workshops is to humanize the high school chemistry curriculum and to better communicate the problems and advantages faced by industry in meeting its multiple responsibilities to community, employees, and stockholders;
- Holds the *Ralph Connor Lecture Series* on the development of the chemical process industries (sponsored by the Rohm and Haas company and the William Penn Foundation);
- Sponsors, with the Philadelphia Section of the American Chemical Society, the *Glenn E. Ullyot Public Affairs Lecture Series*, aimed at exploring the impact of the chemical sciences on society;
- Sponsors, with the American Chemical Society, a *National Landmarks* program to identify, publicize, and preserve manufacturing sites, equipment, homes of chemists, etc., that are of vital importance to the history of the chemical sciences;
- Conducts (and has completed over 100) extensive interviews with leading chemical scientists and industrialists;
- Organizes *Conversazioni*, social occasions to introduce leaders in the chemical industry and their friends to the Foundation and its friends;
- Publishes *Chemical Heritage*, currently a 32-page magazine which brings alive the story of chemical achievement to a readership of over 20 000 worldwide;
- Publishes annually (with the American Chemical Society) *Milestones in Chemistry*, a color-illustrated calendar of particular interest to school children and teachers which marks dates of discoveries, birthdays of chemical scientists, etc.;
- Publishes paperback books and pamphlets on such topics as:
  - *American Chemical Enterprise;*
  - *The Value of History;*
  - *The History of Chemical Instrumentation;*
  - *Electrochemistry, a Science at the Interface;*
  - *What is Oral History?;*
  - *The First Century of Chemical Engineering Polymer Pioneers.*

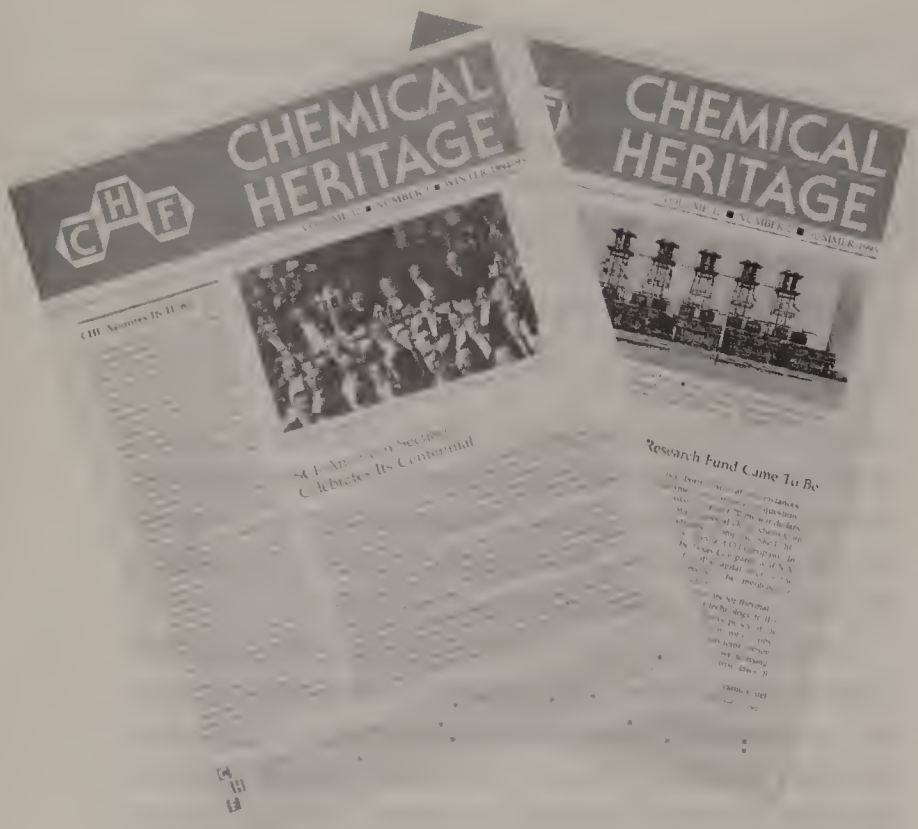


Fig. 1 Chemical Heritage is the magazine of the Chemical Heritage Foundation.

The Center's work also includes a variety of scholarly projects and events of interest to the academic community, such as:

- A sustained inquiry into the development of polymer science and technology in the twentieth century;
- The *Biomolecular Sciences Initiative* – recording history as it happens from the rise of molecular biology some fifty years ago to the contemporary efforts to map the human genome;
- The *Edelstein International Fellowships and Studentships*, which fund two scholars each year to do basic historical research at the Center and at the Hebrew University of Jerusalem;
- A program of small travel grants to scholars working at the Center;
- A monograph series on '*The Chemical Sciences in Society*' (copublished with the University of Pennsylvania) including:
  - Peter J. T. Morris, *The American Synthetic Rubber Research Program*;
  - Fred Aftalion, *A History of the International Chemical Industry*;
  - Seymour H. Mauskopf, editor, *Chemical Sciences in the Modern World*;
- A series of reference books and popular works, copublished with the American Chemical Society, such as:
  - Laylin K. James, editor, *Nobel Laureates in Chemistry 1901–1992/1993*;
  - Theodor Benfey and Peter J.T. Morris, editors, *Robert B. Woodward. Scientist and Artist in the World of Molecules*, 1995;
- Development of basic research tools for chemical history, such as: George Tselos and Colleen Wickey, *A Guide to Archives and Manuscript Collections in the History of Chemistry and Chemical Technology*, 1987;
- Symposia and conferences on subjects such as commercial applications of developments in organic chemistry, and the development of modern chemical instrumentation.

In its academic programs, the Beckman Center works closely with the Department of History and Sociology of Science and with the Departments of Chemistry, Chemical Engineering, and Biochemistry, and with the *Laboratory for Research on the Structure of Matter* at the University of Pennsylvania, as well as with other research universities.

The Othmer Library was founded in 1988 when Donald F. and Mildred Topp Othmer announced a challenge grant 'to create a library commensurate with the achievements of the chemical sciences and industries.' Steps toward this goal include a donation from The Chemists' Club of more than 10 000 books and over 20 000 volumes of journals spanning the era from the American Civil War (1861–1865) through World War II, a purchase of 1000 rare books from the library of the Franklin Institute, and major donations from the Brooklyn College of Pharmacy, Long Island University, and the *Société de Chimie Industrielle*. The Othmer Library's collections continue to expand significantly through donations from individuals and chemical organizations.

The Library promotes access to materials on the origins, development, and current directions of the chemical sciences and technologies by:

- Maintaining a comprehensive reference collection;
- Developing special book, manuscript, and oral history collections;
- Collecting papers of chemical scientists and organizations;
- Collecting key chemical instruments in its museum;
- Providing database entry to other historical collections.

The Othmer Library currently houses approximately 20 000 volumes in its stacks and 1300 volumes in its reading room, as well as archival materials, selected serials, audiovisual materials, artifacts, ephemera, and non-print materials. The collections are subdivided into (1) Books (comprised of the Core and Reading Room Collections, Historical Textbook Collection, BIMOSI and Oral History Collections, and Old/Rare Books); (2) Serials; (3) Vertical Files (including corporate history and biographical files); (4) Audiovisual materials; (5) Archives (comprised of the papers of eminent chemists including Carl Marvel, William J. Bailey, Nobel Laureate Paul Flory, and industrial chemist and Lexan inventor Daniel Fox, as well as the archives of professional organizations such as: The American Institute of Chemists, The Electrochemical Society, Inc., and several

divisions of the American Chemical Society); (6) Oral History Files and Transcripts (which includes 115 completed interviews and 70 completed transcripts); (7) Pictorial Collection (including over 2000 prints, negatives, slides, and ephemera of chemists and engineers, and of laboratories, chemical plants, etc.); and (8) Artifacts, including several early pH meters and spectrophotometers. Among the Othmer Library's rare-book holdings are Lazarus Ercker's *Bergwerksbuch* (1598), Robert Boyle's *Usefulness of Experimental Natural Philosophy* (1664), and Humphry Davy's *Elements of Agricultural Chemistry* (1813).

Although still in its infancy, the Library provides collection management, donation administration, and reference services on a regular basis. Current space allows for the shelving of only one-fourth of the Othmer Library total collections. Although adequate when originally occupied, this space no longer meets the Chemical Heritage Foundation's need, nor the Library's projected growth to 250 000 volumes, and a major artifact collection over the next 15 years. It is anticipated that a total of 10 000 net square feet of library space (30 000 linear feet of shelf space) will be required for the Othmer Library's immediate future.

OLOCH's Museum

During the last half century, the United States has led the world in scientific instrumentation through technological advances which have revolutionized laboratory techniques and industrial operations and led to such exciting breakthroughs as the Human Genome Initiative. As chemical instrumentation continues to advance, older instruments are being discarded. Thus, we have the opportunity to collect these instruments as witnesses to the history of innovation, and also to develop a new resource for advancing the public understanding of science.

There now exists a proposal within the chemical community (sparked by the joint efforts of the Antiquity Museum of the 1994 Pittsburgh Conference and an *ad hoc* committee within the Society of Applied Spectroscopy) to found a museum. The Chemical Heritage Foundation, in collaboration with the Society of Applied Spectroscopy, have created the Chemical Instrumentation Museum Group (CIMG) as a component of the Chemical Heritage foundation's Othmer Library. The Chemical Instrumentation Museum group has been charged with the responsibility of establishing such a museum. CIMG's mission statement points to the significance of such subjects as spectroscopy, Nuclear Magnetic Resonance (NMR), X-rays, chromatography, process control, etc. One aim of the Museum will be to show how instruments of measurement and control have played a vital role in the development of science and industry.

Since its inception, the Foundation has ben located on the campus of the University of Pennsylvania. The Chemical heritage Foundation currently rents from the University about 5000 square feet in a modern building at 3401 Walnut Street. Although adequate when originally occupied, this space no longer meets the Foundation's needs.

Following several years of investigation, the Foundation's Site Committee has recommeded that the new home for the Chemical Heritage Foundation be 315 Chestnut Street, at Independence National Historic Park, Philadelphia.

Independence National Historic Park draws about 1.5 million visitors each year. Not only will this potential audience give the Chemical Heritage Foundation a natural opportunity to extend its public outreach through its museum, but the site also lends itself to programmatic collaborations with such institutions as the Americal Philosophical Society. The site adjoins Benjamin Franklin's home (a Federal Museum) and the visitor center of Independence National Historical Park.

The Chemical Heritage Foundation is curently faced with an exciting opportunity. Donald F. Othmer of Brooklyn, New York, has pledged to match, 1:1, funds raised towards the purchase and renovation of the building in which to expand and operate the Chemical Heritage Foundation and its Othmer Library of Chemical History. This opportunity not only allows for the development of a world-class library and museum – it also makes possible the creation of a unique resource through which the chemical community can foster public understanding of our heritage and our future.

Further information about the Chemical Heritage Foundation may be obtained by contacting: The Chemical Heritage Foundation, 3401 Walnut Street, Suite 460B, Philadelphia, PA 19104-6228, USA, Tel.: 215 8984896; Fax: 215 8983327

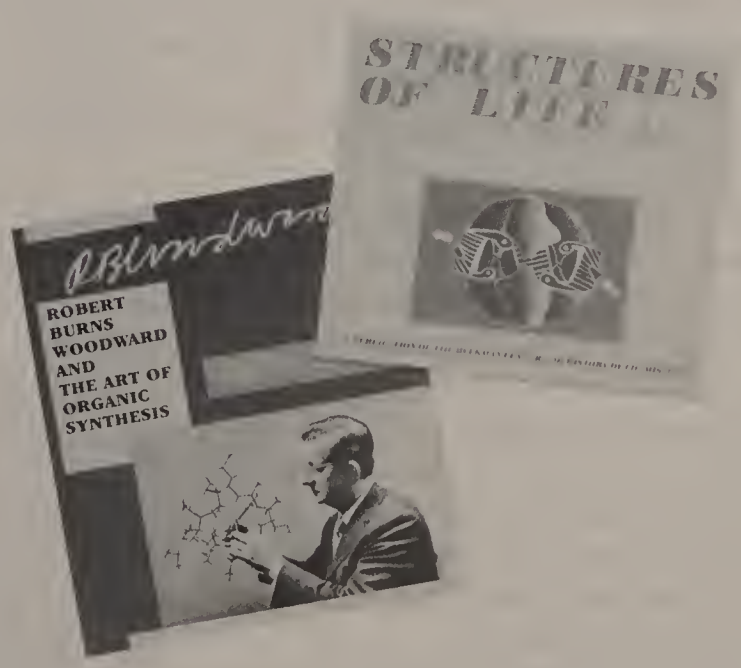


Fig. 2 Examples of the publications of the Chemical Heritage Foundation

What is Happening in Organic Chemistry?

Professors Paul Wender (Stanford University, California, USA), Barry Sharpless (Scripp's Research Institute, California, USA) and Derek Barton (Texas A & M University, Texas, USA) recently attended the Tenth International Conference on Organic Synthesis, Bangalore, India, on 11–16 December 1994. During the conference, these three eminent organic chemists were interviewed by Dr Subbiah Arunachalam, INSA Visiting fellow at the Indian Institute of Science, about their thoughts on current developments and future prospects of organic chemistry. Excerpts of these interviews are given below.

Science: Making the Impossible Possible
Face to face with Prof. Paul A Wender

Professor Paul Wender, the eminent Stanford organic chemist and educator, was recently in India to speak at the Tenth International Conference on Organic Synthesis, held at Bangalore in mid-December.

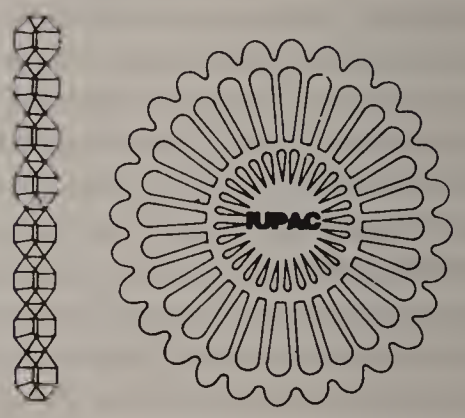
Arunachalam (Arun): How is organic chemistry doing? What is its general state of health?

Paul Wender (PW): These are exciting times for organic chemists. There are opportunities aplenty and indeed the potential for new advances is enormous. Science has been evolving for centuries and with each generation the problems that it addresses have gotten increasingly difficult. Ultimately, our ability to address these problems is determined by our understanding on their molecular origin. Organic chemistry is expected to play a central role in advances of great significance for diverse areas of human activity such as medicine and healthcare, materials, environment and so on. Right now we are undertaking problems of great importance and significance. I would say we are doing well, and our science is healthy. Many institutions are contributing to our subject. Places which are traditionally known for good work are flourishing and several places which have not had a great tradition are also beginning to do well and are coming of age.

Arun: What major breakthroughs are likely in the next few years?

PW: I think organic chemistry will have a tremendous impact on our understanding of various diseases. Soon we should be able to understand cell function — the very essence of life processes. Organic chemistry will also have a significant impact on materials such as new polymers and composites. There is also the potential, although not immediate, for improvements of our environment. Take, for example, the air pollution in Bangalore, or for that matter any city in the world. A catalytic converter can make a lot of difference in quality of life and in health.

Arun: In what ways is organic chemistry of today different from organic chemistry of previous years?



PW: Organic chemical research today is driven by sophisticated theories and instrumentation. Thanks to the rich legacy of theories, instruments and techniques which we inherited from generations of organic chemists, today we can address and in many cases solve problems of immense complexity. Problems that would have taken months for a highly skilled professional only a few years ago can now be routinely handled in a few minutes by a technician or a new graduate student. For instance, Prof. Robert Woodward said in the fifties that the synthesis of erythronolide (a macrocyclic antibiotic) would be difficult if not impossible, but such syntheses are routinely being done today. Things are changing rather rapidly. Organic chemistry now is a central science and a global science with people from many parts of the world working as a single community.

Arun: What is the state of the relation between theory and experiment in organic chemistry today? Is theory able to predict (and help carry out) difficult syntheses?

PW: I should say the relation is healthy. The field is in its infancy and productive interplay between theory and practice has already begun. More and more people use theory now as a tool for moving forward. There is certain amount of scepticism; organic chemists are, by and large, a critical community and this attitude is good for future development. The investments made in theory so far have begun paying dividends. For example, we started using computers in my own lab in 1978. It then took us the better part of a day or even more to merely enter the problem into the computer. Now it takes a student just about five minutes!

Arun: What role do you envisage for the chemical societies of the world?

PW: They should take a greater interest in higher education in chemistry. The institution of education is one of the most beautiful manifestations of the human spirit. It is an invention of our civilization that is dedicated to making the future better – to giving each new generation an opportunity to move forward, to create a better world. Higher education is of singular importance. It should be given the highest priority by chemical societies as well as any government that is truly dedicated to improving the human condition.

Arun: What have chemists done to improve the public understanding of science in general and chemistry in particular?

PW: Not as much as they could be doing, unfortunately. Chemistry is one of the earliest sciences and there is so much of interest and relevance to the public. Journalists could do a great deal. For example, when the taxol stories broke, our laboratory received many positive enquiries from the general public. Someone whose brother or sister was suffering from cancer could immediately relate to the discovery.

Arun: The trend in all fields now seems to be greater interdisciplinary and vanishing borders. Is it true of organic chemistry as well?

PW: I think other disciplines are moving towards organic chemistry! I am a bit chauvinistic about this, of course! Organic chemistry is about three things, structure, change in structure, and new structure: and these areas of expertise will have a major impact in many other fields.

Arun: Has there been much improvement in the teaching of organic chemistry?

PW: There has been a lot of improvement and we can justifiably pat ourselves on our backs. As an academic I am greatly concerned with the training of the next generation of chemists. I want to convey the excitement of chemistry. I am afraid some teachers tend to emphasise nomenclature at the cost of conveying the basic principles and the essential beauty of it all. Chemistry has the logic of mathematics and the utility of other branches of science. There are the challenges; for example, we cannot truly portray the three-dimensional structure of a molecule on a two-dimensional blackboard or paper. We need to use 3-D graphics, visual images, animation and even holography. With the technologies available, soon we should be able to display a huge molecule inside the class room, and students could walk through it! I teach an undergraduate course, in the first lecture I tell the students that all of organic chemistry is essentially reduced to seven concepts: the sigma bond, the pi bond, the steric problem (because molecules have size), the polarization phenomenon (because molecules have charge), the resonance phenomenon, kinetics and thermodynamics. I try to relate the chemistry that they learn to things that they meet with in their day-to-day life. For example, when introducing acid-base theory, I ask them why is seafood always served with lemon. Then I bring a big fish into the classroom and make everyone smell it. The offensive odour of an unrefrigerated fish comes from two amines. Their systematic chemical names do not reveal a thing about their odour. However, their trivial

Bangalore

names, putrecine and cadaverine, are enough to put anyone off. Then I take the fish back to the table, chop it and sprinkle lemon juice on it. Now the amines are converted to a salt and there is no more evaporation of the foul-smelling gaseous amines. The chopped fish is now passed around and no one makes faces. I tell you it is a great experience when the students go and eat at the cafeteria and when they have their fish they tell others about the chemistry behind it all! In the process, they review their lecture and teach others about science.

The most important thing in teaching is to teach your students to teach themselves. As a teacher, I think my job is to nurture the enthusiasm and vigour of every student, help him realise his incredible potential and, in short, empower him. After all, students are our future.

The Return of the Small Molecules: *Face to face with Prof. K. B. Sharpless*

Prof. K Barry Sharpless, one of the world's outstanding organic chemists and the inventor of the Sharpless epoxidation and selective hydroxylation reactions, was in India recently to deliver a special lecture at the Tenth International Conference on Organic Synthesis.

Arun: How is organic chemistry doing? How is its general state of health?

KBS: Organic chemistry has gone through a difficult period in recent years compared to the last generation. It had to face stiff competition from biochemistry and biology, both of which had become much more exciting than ever before. But biotechnology has been a bit of a failure; at least it has been a disappointment; it promised so much, but did not deliver. Now people in the pharmaceutical industry are going back to small molecules, and I think organic synthesis has a very big role to play in the future of medicine. There is so much unexplored chemical diversity, I would say that we have not seen anything yet. So far, we have exploited only a very tiny part of the variability. Unfortunately, we have been trying to make too many carbon–carbon bonds; it is simply impractical. It takes so much effort to make molecules with long runs of continuous carbon–carbon bonds. Nature makes virtually all its large, information-rich structures as oligomers of small units linked by heteroatoms. Now, using solid phase reactions one could build many types of scaffolds and different structures useful in making new materials, separations, drugs and those which are biologically active. Indeed, starting from one hundred carbon atoms, 40 or 50 nitrogen atoms, 40 or 50 oxygen atoms, etc., one could make so many different species of molecules that their combined mass would be astronomical, and > 99.9999% of them would be 'new' compounds. Currently there are at least ten small companies in the USA dedicated to making such small molecules combinatorially, and most of the major pharmaceutical companies have their own programmes in this area.

Arun: What major breakthroughs are likely to take place in the next few years?

KBS: There has been much interest in drug design in the recent past. I don't think rational drug design will be all that successful. I feel intelligent and intuitive screening is the best approach. I think asymmetric synthesis, sophisticated specialty polymers, and efficient multi-component coupling are some of the promising areas. I think the diversity approach to making new and new combinations of molecules will be to the fore. For the latter purpose, we need more and better reactions, reactions fueling the chemical diversity craze, reactions that work most of the time and give yields of 95% or more.

Arun: In what way is organic chemistry of today different from organic chemistry of previous years?

KBS: A whole generation of organic chemists were so tied up with synthesizing big natural products. Nothing wrong in that, except they were all after synthesizing specific molecules that were found in nature and developing methods which were generally too specialized to be of wide significance.

I think there has always been a strong reverence for the chemistry of life among organic chemists. In fact, vitalism is not yet dead. So a lot of people are trapped into that kind of a box canyon! I would not say that their efforts are lacking in merit. It certainly trains people for synthetic work. I would say they had not looked over their shoulders enough to see the wider opportunity to develop general reactions that would work more reliably to make molecules having the desired properties in a much faster and more economical way. For lack of imagination, many people have been synthesizing polypeptides as an approach to chemical diversity. But polypeptides are no good for drugs; they get hydrolysed.

Arun: How do you judge good work in organic chemistry?

KBS: I will go by the criterion of 'new reactivity' . Work reporting a new or improved reaction which is faster and more efficient is good. In my own group, we try to engineer high selectivity into known reactions. In my view, long, multi-step synthesis of large molecules, however elegant it may be, is of limited value, and is one of the least efficient ways to uncover important new reactivity.

Arun: Your impressions of organic chemistry in India, please.

KBS: Indian chemistry is even more vigorous than I expected. The synthetic organic chemistry here is very practically oriented, so it is poised to take full advantage of the explosive growth I predict for India's pharmaceutical and fine chemical industry.

In search of more efficient reactions: *An interview with Prof. Derek H. R. Barton*

Prof. D H. R. Barton, winner of the 1969 Nobel Prize for chemistry for his work on conformational analysis and one of the most perceptive of organic chemists, was in Bangalore recently to give the inaugural lecture at the Tenth International Conference on Organic Synthesis. An elder statesman among chemists and a Fellow of many national Academies of Science including the Indian and the Chinese, Prof. Barton is well known for his many contributions to the development of new synthetic methods and the discovery of many new reagents for selective organic transformation and deoxygenation via radical intermediates.

Arun: What major breakthroughs are likely in the next few years?

DHRB: If I knew them I wouldn't be talking about them; I would be making them happen in the lab! I expect major advances in highly stereoselective saturated hydrocarbon oxidation. Unlike unsaturated compounds, oxidation of saturated hydrocarbons is rather difficult.

Arun: In what ways is organic chemistry of today different from organic chemistry of previous years?

DHRB: The philosophy has not changed, only there have been improvements in the tools and concepts. The aim continues to seek the order that exists in nature and to impose our will on it. The major challenges have not disappeared. For instance, 100% yield is still a distant dream.

Ideally, a new reaction should give 100% yield of a single product at room temperature and preferably under neutral conditions and atmospheric pressure.

Arun: What is the state of the relation between theory and experiment in organic chemistry?

DHRB: Theory has always followed experiment. It provides an explanation after the event. Hardly ever has theory predicted experimental results. Nobody ever predicted ferrocene or fullerene. But it seems much easier to publish a paper reporting calculations than to publish a real chemistry paper!

Arun: What role do you envisage for the chemical societies of the world?

DHRB: They already publish journals and organise meetings. They should continue to do that. They should help younger chemists; they could charge a lower fee, for example.

Dr Subbiah Arunachalam is an information scientist, science writer and editor. He is currently with the Central Electrochemical Research Institute, Karaikudi, India. His research interests are in the fields of information access and scientometrics. Dr Subbiah Arunachalam is a member of both of the International and the Indian Science Writers Association, and has conducted many workshops for science writers.

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Appl. Chem.*

Some problems in the destruction of chemical munitions, and recommendations towards their amelioration (Technical Report)

These recommendations are offered primarily to national authorities with responsibility to destroy chemical munitions and the chemical warfare (CW) agents they contain. They probably also will be of interest to citizens who are in one way or another concerned with this question. The problems and pertinent recommendations are as follows:

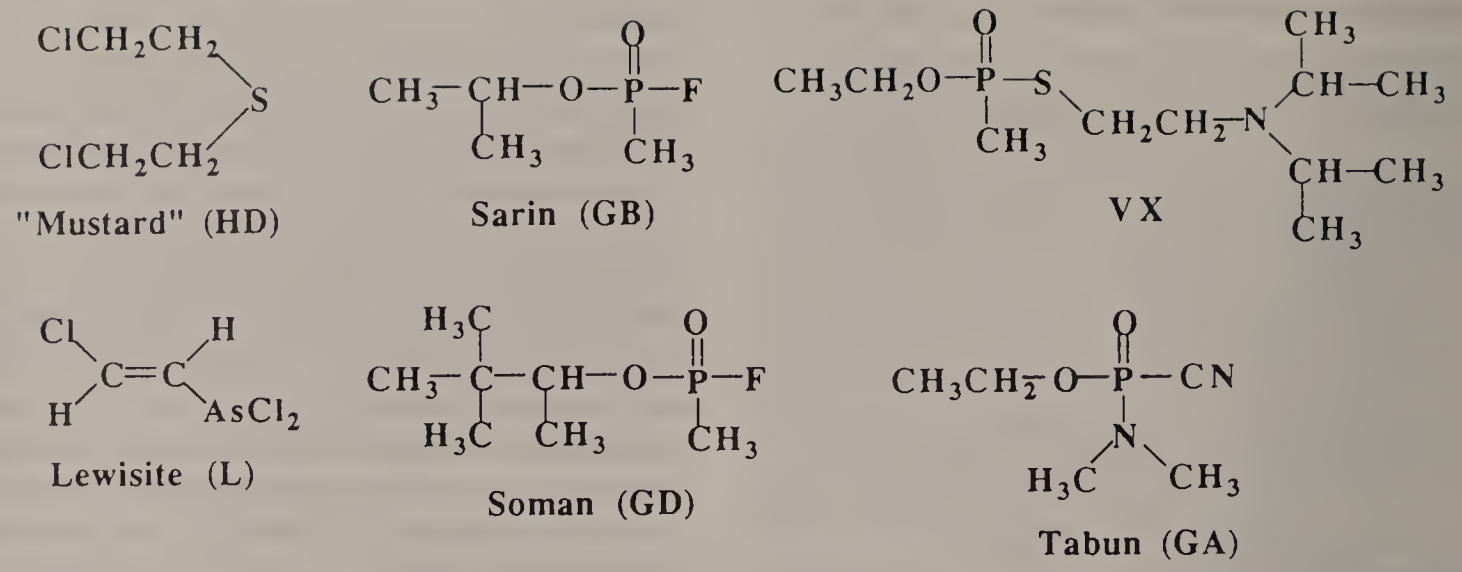
A. Problems of Science and Technology

(I) How long do chemical warfare agents linger in the environment, and what happens to them? *Recommendation*: Investigation of rates and products of degradation of chemical warfare agents in the environment and under relevant controlled conditions should be undertaken.

(2) The problem of recovered old munitions: what they are, and what is in them? *Recommendation*: Efforts should be made to discover and develop additional useful methods for nonintrusive identification of the contents of recovered old munitions.

(3) The problem of gelled or crusty materials in containers of 'mustard'. *Recommendation*: The chemistry of gelled or crusty HD ('mustard') should be thoroughly studied.

(4) The problem of ascertaining bow much chemical warfare agent may remain after being subjected to a



Principal Modern Chemical Warfare Agents

destruction process. *Recommendation*: Research to discover and develop superior analytical methods for detection and quantitative determination of any CW agent surviving destruction processes should be undertaken, insofar as methods now known are less than fully satisfactory.

(5) The problem of monitoring of air spaces and gas streams during storage and destruction of chemical warfare agents. *Recommendation*: Further research toward, and development of sensitive, definitive methods and equipment for rapid monitoring of air spaces and gas streams should be undertaken.

(6) The problem of inadequacy of knowledge about the fundamental chemistry of chemical warfare agents. *Recommendation*: Rigorous research for systematic expansion of knowledge of the fundamental chemistry of chemical warfare agents, as relevant to their destruction, should be conducted.

(7) The problem of disposal of scrubber or neutralization brines. *Recommendation*: Scientific questions raised by possible ocean discharge of refined brines resulting from destruction of chemical warfare agents should be investigated.

(8) The possibility of combining destruction of a chemical warfare agent by 'neutralization' with follow-up degradation of the intermediate products by wet air or supercritical water oxidation. *Recommendation*: The feasibility of combining neutralization with ensuing wet air or supercritical water oxidation into an integrated process should be studied, with special attention to engineering concerns.

B. Problems of Information and Communication

(1) The problem that the lay public is not adequately informed about technological aspects of the destruction of chemical weapons. *Recommendation*: Chemists are urged to communicate with their fellow citizens by writing articles in language intelligible to laymen, by giving public talks, and by participating in radio and television broadcasts.

(2) The problem that some studies of the properties and chemical reactions of CW agents, relevant to their destruction, which were militarily secret during the Cold War, have not been made publicly available. *Recommendation*: The chemists who did those studies or department heads who have custody of their reports are urged to make them available to aid scientists of the world in one of three ways: *preferably*, by publication in peer-reviewed scientific journals; *alternatively*, as publicly available reports; or (for minor studies of good quality) by submission to the Technical Secretariat of the Organization for the Prohibition of Chemical Weapons, for inclusion in a data bank.

(3) Problems of locating existing publications. *Recommendation*: A comprehensive bibliography of published or publicly available reports concerning properties and chemical behavior of CW agents relevant to their destruction, to be available to all persons in all counties on payment of a modest charge, should be prepared.

This report was prepared for publication by Prof. J. F. Bunnett, Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA 95064, USA, for the Taskforce on Scientific Aspects of the Destruction of Chemical Warfare Agents, in the Organic Chemistry Division. The full details are published in Pure & Appl. Chem. ***67****, 841–858 (1995).*

A note on the work of the Taskforce can be found in *Chem. Int.* **17**(2) 52–56 (1995).

Commission & Committee News

Minutes of the meeting of the Commission on Water Chemistry, VI.6, Belgirate, Italy, 11 September 1994

Projects

Review of progress of existing projects.

In-situ *Treatment of groundwater*
The final draft is ready and was circulated among the Commission members who were invited to comment on the draft.

Workshop on Quantitative Structure Biodegradability Relationships (QSBRs)
Preparations for the workshop have been completed, the workshop was organized on 12 September 1994. The proceedings of the workshop will be published in SAR and QSAR in Environmental Sciences. Also they will be distributed among participants, members of the Water Chemistry Commission and other scientists who are interested.

Immunoassays for Water Monitoring
A draft paper has been prepared. During the meeting it was suggested to include the use of immunoassays for screening purposes (for instance pesticides in drinking water).

Atmospheric Chemistry and Distribution of HCFCs Oxidation Products in the Hydrosphere
Since no significant input from within the Commission is expected to be generated in the near future, it was proposed to terminate this project.

Code of Practice for reporting analytical data for environmental samples
An explanation was given by Dr Dobbs on progress of this project. It is intended to come out with recommendations on the information that needs to be submitted when reporting analytical data. A draft was prepared on 'Code of practice for reporting data for fish tissue'. Dr Dobbs will reprocess the draft and contact SETAC for further information. One of the items to be discussed is possible overlap of activities.

It was agreed that, before the next meeting, Dr Carter and Dr Kördel will prepare an outline on a similar project relating to soil chemistry.

The importance of natural organic material for environmental processes in waters and soils
An outline on this project was prepared by Dr Kördel and sent to Dr Lintelmann, Dr Wright, Dr Rodrigues de Aquino and Dr Dasenakis. Dr Lintelmann and Dr Dasenakis agreed to cooperate. Dr Dasenakis will concentrate on the marine part, and Dr Lintelmann on freshwater ecosystems and analytical aspects. The input of an extra soil chemist is needed. Perhaps a member from the pesticide commission can assist. Dr Kördel will contact the chairman of this commission.

Concern of overlap with the activities of other commissions has been expressed by the officers of IUPAC. Dr Dobbs will respond by stating that there is no ground for concern: there is no duplication of activities

A joint project is planned to be carried out with the Atmospheric Chemistry Commission on the impact of deposition of nutrients on ground water quality. At the moment various similar initiatives seem to be under way in Europe. Dr J. Slanina, the project coordinator for the Atmospheric Chemistry Commission, wants to inventory what is going on and after that he will decide on how to proceed. Dr Slanina will contact Dr Carter as soon as a decision on how to proceed with the project, has been made. When something has been decided, Dr Carter will report to the other Commission members.

Feasibility studies

Disinfectant Residuals Measurement. No progress was made. Early in 1995 it will be decided whether sufficient information will become available to allow continuing this project.

Hydrology/Chemistry Terminology. An Israeli scientist will be contacted by Dr Shevah in order to be able to decide on the best approach for this project.

Sediment Interstitial Water Interactions. At the next General Assembly it will be decided what will be done in this area.

Chemical Processes in Membranes for Environmental Protection Purposes. The basis of the project will be the use of dynamic membranes for brackish water desalination. Dr Shevah will contact Prof. Grebenjuk to prepare a proposal for a project.

Henry's Law and Environmental Processes. Dr Peijnenburg will contact the coordinator of the Atmospheric Chemistry Commission.

The Chemical Properties of Sewage Sludge. The idea behind this study is to review the composition of sewage sludge from a chemical point of view. Information published will be exchanged and a suitable topic will be selected. Dr Carter will ask an MSc Student to prepare a literature review. All members are requested to send relevant information to Dr Carter.

Proposals for new projects

Several suggestions for new projects were put forward. These include:

- Sediments: Environmental impacts of remediation.
- Bioavailability: At the next meeting Dr Peijnenburg will propose a structure for a feasibility study.
- Control of remediated soils. Dr Kördel will propose a structure for a feasibility study.
- Artificial sediments.
- Dr Carter proposed to undertake a study on 'Solute movements in soils with the potential for rapid bypass movement'. Dr Carter will make sure that there is no overlap with activities within the pesticide commission. It was decided that Dr Carter will prepare a project proposal, which will be sent to the Applied Chemistry Division for consideration. After their approval, Dr Carter will be the project leader of this project.

The next meeting of the Commission will be held during the IUPAC General Assembly on 4–7 August 1995 in Guildford (UK).

W. Peijnenburg,

Secretary, IUPAC Commission on Water Chemistry.

Minutes of the meeting of the Commission on Solubility Data, V.8, Buenos Aires, Argentina, 20–21 August 1994

Report of the Chairman (M. Salomon)

The Franzosini Award

Dr Salomon announced that the recipient of the award for 1994 was Dr Erich Königsberger (Montan Universitat, Leoben, Austria). This award assisted Dr Konigsberger in attending the meeting in Buenos Aires. Recommendations for the 1995 award should be sent to Dr Salomon.

Activities within IUPAC

Dr Salomon reported that after deliberations on restructuring, the number of Titular Members on Commission V.8 was now reduced to six and there was a possibility of a further reduction. This action would definitely create problems in the future as the travel budget for such a large Commission is already strained to the limit.

The general idea of the restructuring was to create a pool of Titular Members with four members being allocated to each division so that Limited Lifetime Commissions (LLTC) could be established to work on topical problems. It is proposed that such special Commission projects would last from 2 to 4 years. Professor A. Hulanicki (Chairman, Analytical Chemistry Division) favoured the creation of a LLT Commission on Macrocyclic Ligands in Cooperation with the Commission on Equilibrium Data (V.6).

Dr Salomon then led a discussion related to the visibility of the work of Commission V.8 both within and outside IUPAC. It was felt that our work is not well understood by IUPAC. It was agreed that we need to prepare some background information on the Solubility Data Series which outlines the objectives, the accomplishments and focuses on important applications of the work and also includes a general overall plan of action. We need some coverage in magazines such as *Chemical and Engineering News* (the weekly ACS publication) and *Chemistry International* and other publications published by Chemical Societies in various countries. A committee formed from the Sub Committee Chairpersons will prepare relevant information by December 31, 1994. Professor Lorimer agreed to serve as the editor for the material. Input from any members of the Commission is encouraged. The information obtained would also be used for potential contributors to the project as well as for the consumers.

Solubility Database Project (D. Shaw)

At the meeting in Lisbon a working party consisting of F. Getzen, A. Maczynski, D. Shaw (Chair) and A. Skrzecz was appointed to develop standard ASCII file formats for the electronic storage of compiled & evaluated solubility data.

In June 1994, the working party circulated information about the file formats that had been developed. After receiving comments, draft guidelines containing specific directions for electronic data format have been completed. The material contains about 50 examples. Further suggestions are needed for refinement. The final draft of the recommendations is scheduled for November 1994. After approval by Dr Salomon in consultation with other members of the Commission, their recommendations will be submitted to the Committee for Chemical Databases (CCDB) by February 1995 for their consideration at the next General Assembly meeting at the University of Surrey in August 1995. It is expected that the CCDB will suggest possible databases.

In the course of the discussions led by Professor Shaw, it was strongly recommended that all future volumes of the SDS should be accompanied by electronic storage (data archive). There should be a clause in the contract with OUP that they will accept computer based volumes which they can print if required. Also, material from the data archive could be abstracted for future databases.

Horizontal Programs

Solubility of Gases in Aerosols (P. G. T. Fogg)
Dr Fogg reported on discussions with Prof. P. Warneck (Commission VI.4, Atmospheric Chemistry) and confirmed the interest in collaborative efforts between the two Commissions. At the Commission meeting in Buenos Aires it was agreed that preliminary work should be started on a proposed project entitled: 'Solubility of Vapors of Liquids Boiling above 298K'. The initial effort will be confined to the evaluation of solubilities of vapors in pure water and sea water. A preliminary literature survey will be carried out during the next few months to determine the extent of the data that are available so that the project can be planned in detail. It is expected that most of the relevant data will be in the form of partial vapor pressure measurements on solutions of organic liquids in water. Solubilities of organic vapors of environmental importance will be given high priority. The status of the proposed project will be discussed at the next Commission meeting at the IUPAC General Assembly in August 1995.

Solubilities and Thermodynamics of Macrocyclic Ligands (A. F. Danil de Namor)
Dr Namor discussed plans for a cooperative project between Commission V.8 and V.6 on Macrocyclic Ligands. One proposed volume will contain solubility and thermodynamic data for all macrocyclic ligands. Solubility data would be the responsibility of Commission V.8 while the equilibrium data such as enthalpies of complexation and heat capacities would be undertaken by Commission V.6. A recommendation was made to prepare a special volume (monograph) outside the normal SDS series. This recommendation was approved. It was suggested that data for 18-crown-6 should be compiled, together with evaluations as an example of a macrocyclic ligand where a large amount of information exists.

Sixth International Symposium on Solubility Phenomena (A. Danil de Namor)

Dr Namor reported on the status of the Sixth International Symposium on Solubility Phenomena which was held immediately after the Commission meeting (22–26 August 1994) at the Hotel Bauen, Buenos Aires, Argentina. Approximately 90 delegates were expected to attend, including 23 scientists from Argentina and three from Mexico. The Scientific Program consisted of nine plenary lectures and seven invited lectures. A poster session had 24 presentations. There were also 21 contributed papers. Sponsorship for the conference had been difficult. The European Union and IUPAC provided a large fraction of the financial support which was used to assist scientists for travel to the conference. Also the Soros Foundation provided support for a number of Russian and Bulgarian colleagues.

Future International Symposium on Solubility Phenomena

Seventh International Symposium on Solubility Phenomena (H. Gamsjäger)
Dr Gamsjäger reported that the Seventh International Symposium on Solubility Phenomena will be held on 22–26 July 1996 at Montanuniversitat, Leoben, Austria. A meeting of the Solubility Data Commission will be held immediately before the Symposium on 20–21 July 1996.

Dr Gamsjäger proposed a conference program which was a balance between established and popular themes together with some new fields such as Solubility and Metallurgy. Drs. P. Fogg and E. Waghorne were appointed as conference editors. The first circular announcing the conference will be ready in November 1994. Some suggestions for Plenary and Invited Lectures have already been made. Additional input is needed.

The 21st meeting of the IUPAC Commission V.8 will take place during the 38th IUPAC General Assembly at the University of Surrey, Guildford, UK on 5–7 August 1995. Your participation is urgently requested.

R. P. T. Tomkins (Secretary)

Minutes of the meeting of the IUPAC Committee on Chemical Databases, CCDB, London, UK, 4 December 1994

CCDB Chairman's Visits to Oxford and the Committee's New Terms of Reference

Terms of Reference for the Chemical Database Committee have been altered by IUPAC Secretariat. They were changed so that the committee would have the responsibility to help coordinate the computer environment and recommend changes as required to keep the secretariat's office operating smoothly. Dr Heller's last visit to the secretariat's office revealed a number of difficulties with their current operating environment Dr Heller also noted that some of the difficulties they were having should be able to be resolved with a little effort on the part of CCDB. After some discussion, CCDB members felt that assistance was needed beyond what the current IUPAC consultant had been offering. Members of the Committee agreed, and it was suggested that a letter be drafted by Heller with some recommendations and an offer to help try to straighten out their current environment.

Future of the CCDB

There have been continuing discussions on the merging of the CCDB with the Publications Committee to form a single body. The expanded Committee would view publications not as books, but also potentially as databases or other electronic media. Heller reported that there had been discussions with Dr Bowen (Chairman of the Publications Committee) and Dr M. Williams as well as with Dr Becker (who is retiring as the Chairman of the Publications Committee at the end of 1994) . A proposed new Terms of Reference was discussed as well as possibly giving this committee a new name such as Information Strategy and Technology Committee. It was the sense of the CCDB that the merger should be recommended and that the committee should be made up of a chairman, a vice chairman, plus six full members, and between zero to three affiliates. (CCDB felt that this represents the movement in the entire community with technology forcing change from print to electronic forms, and this merger is really just reflecting that change.

Progress on Databases

Entvapor
Nothing new to report.

Stability Constants
Dr and Mrs. Petit distributed a report.

The complete database from 1974 to 1989 is now loaded. Also, about 100 copies have been sold. By the time of the General Assembly meeting in Guildford, in August, all the data should be loaded (around 250 000 equilibria). A financial statement was given to the chairman and a copy is available in the official records of the committee. The price of this database for academics is GBP250 and about 60% to 75% of the sales have been for academics. The commercial price is GBP375. The Petits believe the database needs a network version, and also needs to be moved to Windows as soon as possible. They are currently supplying multi-user version by giving additional copies. They are also looking at data graphing as added feature.

Solubility Data
There have been no new developments with this database project The project will remain on hold until CCDB is contacted by the Solubility Commission.

IUPAC Recommendations Database
A recommendation to officially thank Dr Jain as well as Dr Kiessling (a former member of CCDB) for all of their work on producing this initial version was approved by CCDB. CCDB recognizes that IUPAC needs to move this project into more of a maintenance mode. At this committee's request, Mrs. Pettit was asked to examine the software. She will look at the system and propose a cost and contract for the on going maintenance of the project. Mrs. Pettit will directly propose a letter of contact with the secretary's office directed to Ms. Troughton to try to get this set-up.

Thermodynamic Properties
Nothing new to report.

Clinical Chemistry Silver Book
Mr. Kaindl did get the book and brought it back to Sandoz to have it evaluated for it's utility. The database format was not optimal to make the data useful. It is also not clear who this book was intended to serve. The commission proposing this project, felt that all the clinical chemistry groups in the world would like to have this. However, the clinical groups at Sandoz certainly did not agree. The book included proposed standards from the IUPAC Commission, but did not appear to be in synchronization with some of the governing authorities such as, US FIDA or others.

Other Databases
Dr Davies asked to check the orange book indexes of the first and second keywords for all the technical committees. Thousands of these have definitions and units. The indexes has been translated into various languages such as Japanese, Chinese, and German. This would be an excellent possibility for a World Wide Web server. We should ask them to produce the next version in computer readable form.

Standard Molecular Data Format Project

Dr Potenzone gave a brief overview of the progress on the Chemical Exchange Format (CXF) file format being developed by Chemical Abstract Service (CAS). The initial version of the format has now been completed and circulated to a wide audience, including all the members of this committee. A number of questions were raised by various members of the CCDB:

- A sketch format such as the clipboard is becoming the de facto standard. Response; While this is true, CXP is a much broader standard that covers the sketch format as well as a variety of others including queries, 3D, reactions etc.
- What formats did we plan to support with CXF Response: CAS will create a few converters, such as

SMILES both input and output. These will be made public in the near future. We hope that others will add to a public collection of these.

- There was also a question of how much user data can be put into this? Response. The format is open and extensible so that it can be expanded as needed. However, user extensions may not be handled correctly by other applications without modification.
- Does CAS own this standard definition? Response: CAS will make this a public format We will continue to maintain the standard but will not require any license or fee for use.
- The format as so complex, will never be used? To what extent will this relate to other standards groups? Response by Dr Jochum: with or without the IUPAC endorsement, if CAS is pushing it, it will be used. Dr Wolman pointed out that whether we endorse it or not, i.e. community will ultimately decide.
- Is there a simplified version of CXF? How will protein such as ATPase fit within this format and will there be a significant increase in file size? How well does the format scale up? Dr Potenzone will respond to this question later.
- How about other formats? Such as the one published by crystallographers in the *Journal of Chemical Information and Computer Science* (JCICS), the star formats? How is this work in any way reflected in the work being proposed by Dr Frank Brown at Glaxo?
- Dr Chihara suggested that we need to be careful especially if individual chemist begin to use it because there is not a simple one to one relationship between one format and another. Starting with a CAS Registry 3 format, going to CXF, and then to a MDL format, and then back to CXF, and then back to Registry 3, what's the chance that we end up with the same representation?

The CCDB concluded that endorsing standards such as this was an excellent purpose for this committee. The CCDB consensus was that CAS needs to formally submit the CXF format to CCDB in order for the CCDB to be able to recommend it for approval. At that point if the committee accepts it, it can forward it to the Executive Committee for approval. There is general consensus that CAS needs to publish a test set of around 200 molecules, especially with chirality included. The tests should be published as a validation study in JCICS, for example. Dr Kaindl commented that this must be a living standard. It will need additions in future both in format, data dictionary, and other new things that may come. In addition to the letter request by Chemical Abstracts, CCDB would like to see some proof of commercial viability. Dr Kaindl would also like to see some contact with potential users.

Dr Rzepa (Imperial College, London) explained his MIME (Multi-purpose Internet Mail Extensions) chemistry extension. He's been working with Dr Peter Murray-Rust from Glaxo and they are in the final stage themselves of proposing a format. MIME is a standard for including information within mail messages they proposed in 1993 with seven primary types of information. All of this has come about in the last 18 months. A chemical MIME must allow all information published in the literature to be included electronically in a document. Dr Rzepa said that he will be writing a proposal to this committee.

IUPAC Internet File Transfer Protocol (FTP)/ Gopher site

CAS is just begnning to make use of the World Wide Web to make its information available and is not prepared at this time to offer these services for the IUPAC proposed projects. Hopefully this will change in the near future.

There was a discussion about asking Derwent if they would be willing to do this. There is also the possibility of going to Darsbury. The other idea was to approach the Oxford Chemistry Department's new Information Technology director, who had just been appointed. It would be usefill to be loaded as mirror sites in, any event, and possibly have all of the proposed sites bring up these files. This will be discussed again further at the Gulidford meeting.

Joint Committee on Atomic and Molecular Physical Data (JCAMP DX) Project

Dr Davies explained that there are proposed IR and NMR data exchange formats actually in use today. IUPAC would be a better place to drive these standards but the spectroscopy commission has effectively rejected this due to structural and financial reasons. ASTM 49.52 committee has been stalled because the binary standards are not very usable and they are looking to find a standard. The question we asked was: What is the role of this committee, if not to publish and accept these standards? Dr Rzepa, speaking with the future of electronic journals in mind, pointed out that this will become even more of an issue in the future. Dr Davies's group would do the work to finish the standards if they are asked to by IUPAC. The committee seemed to feel that IUPAC should endorse this standard and request someone to complete the work. Dr Davies would complete this work at Dortmund at no cost to IUPAC. Dr Heller will write a letter and propose this approach. Assuming that he receives a positive response, Dr Heller will also write to JCAMP to request transfer funds of around $10 000 to a separate IUPAC account. At the Guildford meeting next summer, we will review where we are.

Dr Rudy Potenzone (Secretary)

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in Chemistry International as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional center requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most up-to-data list of the national/regional centers appeared in *Chem.Intl.* **17**, 141 (1995).

Nomenclature for nonlinear chromatography

These recommendations extend the terms and definitions for separations in chromatography which were presented in the Nomenclature for Chromatography (*Pure & Appl. Chemistry*, **65**, 819–872 (1993)) and assumed 'ideal' chromatography and a linear distribution isotherm. However, in practice separations are frequently carried under nonlinear chromatographic conditions in which the distribution isotherm between the stationary and mobile phase is concentration dependent leading to fronting or tailing peaks.

Comments on these recommendations are welcome and should be sent by January 1st 1996 to: Prof. Roger M. Smith, Department of Chemistry, Loughborough University of Technology, Loughborough, Leicestershire, LE11 3TU, UK

In the IUPAC recommendations *Nomenclature for Chromatography*, the conditions under which the chromatography is undertaken are assumed to be purely linear. That is, the equilibrium relationship between the concentration of the sample in the stationary phase C_s, and in the mobile phase C_m, the distribution isotherm, can be expressed as a function $C_s = f.C_m$, if this relation can be written, $C_s = K_c.C_m$ (K_c being a constant of proportionality) then the distribution isotherm is said to be linear. This distribution isotherm can, however, be nonlinear. At low concentrations, all distribution isotherms tend to linearity.

In all types of chromatography, nonlinear effects are common. These are manifest as concentration-dependent retention times and asymmetric elution peaks. Peak asymmetry can, however, arise from other causes. In most applications, nonlinear effects are disadvantageous as they decrease the peak resolution and consequently disturb the quantitative analysis. In preparative chromatography, however, heavy overloading is generally employed in order to increase material throughput, leading to prominent nonlinear effects.

Here, some of the concepts and terms used in nonlinear chromatography are described. It is to be read as a complement to the previously published *Nomenclature for Chromatography*.

Membrane nomenclature

This project has involved assembling a basic set of terms applicable to nonliving membranes and membrane processes. These terms include the key vocabulary used in the literature concerned with scientific, technical and commercial aspects of membrane technology. Processes and membranes based on synthetic or modified natural polymers, together with ceramic and metallic membranes are covered. An initial set of terms and their definitions was revised through mail solicitations of international experts from academia, industry and government. Follow-up solicitations for input were held at four international meetings as poster presentations. The resulting terms and their definitions represent a core set that will allow uniform understanding and eliminate most of the ambiguity and confusion arising from the current use of conflicting terminology. The particular terms and definitions selected for inclusion reflect the majority reflect the majority preference of the community solicited. To avoid irreconcilable differences, definitions and descriptions involving interpretations of phenomena were minimized. Some terms were deleted in cases where majority preferences were not apparent. This strategy was adopted with the understanding that the current core group of terms, which enjoy majority support, may be augmented as the field continues to evolve.

Comments on these recommendations are welcome and should be sent by 1 January 1996 to: Prof. W. J. Koros, Department of Chemical Engineering, CPE Building, University of Texas at Austin, Austin, Texas 78712 USA

Laser-based molecular spectrometry for chemical analysis – luminescence

The various types of molecular luminescence processes have previously been defined in Part VI of the series entitles *Molecular Luminescence Spectroscopy* published in *Pure and Applied Chemistry*, **56** (2) 231–245 (1984). The present document, Part XVI, deals with aspects of laser-based molecular luminescence. Only specific photochemical processes and techniques that take advantage of laser technology are discussed in the present document.

The analytical advantage of laser-based techniques include the high light intensity, monochromaticity, spatial and phase coherence, and the ability to discriminate the homogeneous lines from the inhomogeneous bands. For these reasons, laser-based techniques have become powerful tools in low-temperature and solid-state luminescence spectroscopy.

Comments on these recommendations are welcome and should be sent by 1 January 1996 to: Dr D. S. Moore, Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA.

At room temperature, luminescence spectra of large polyatomic molecules are often observed to poses diffuse structure. In the gas phase, the molecules can rotate and vibrate freely, and a quasicontinum of vibrational rotational lines may be observed as a consequence of the thermal distribution of molecules with the various internal states of the molecules. There is further broadening of the observed lines due to the motion of the molecule and collisions between molecules – Doppler broadening. In solution, by contrast, where free rotations of the molecule are hindered by the presence of the solute molecule, the vibrational structure of the electronic transitions become discrete, however, the individual transitions remain broad. Indeed, the optimal conditions for high resolution spectroscopy on large molecules are obtained at low temperatures, either under equilibrium conditions (translational temperature = rotational temperature = vibrational temperature) in a cryogenic solvent or under nonequilibrium conditions (translational temperature ≠ rotational temperature ≠ vibrational temperature) in a supersonic molecular expansion or beam.

In a supersonic jet expansion, the translational temperature may be reduced by the adiabatic expansion of the gas-phase sample through a small orifice into a vacuum, translational temperatures as low as 1 K and rotational temperature of 5 K may be achieved. At these temperatures, only a few states will be populated and the spectra are consequently much simplified (Fig. 1).

Two types of photochemical process contribute to the spectral width of a particular band in the luminescence spectra of a molecule. First, by virtue of the uncertainty principle, any spectral transition inherently exhibits a certain finite uncertainty in its width related to its lifetime. This inherent contribution to the observed spectral bandwidth is referred to a homogeneous broadening. The homogeneous line corresponds to a transition of a single molecule, and the homogeneous linewidth determines the limit of spectral resolution for that particular transition.

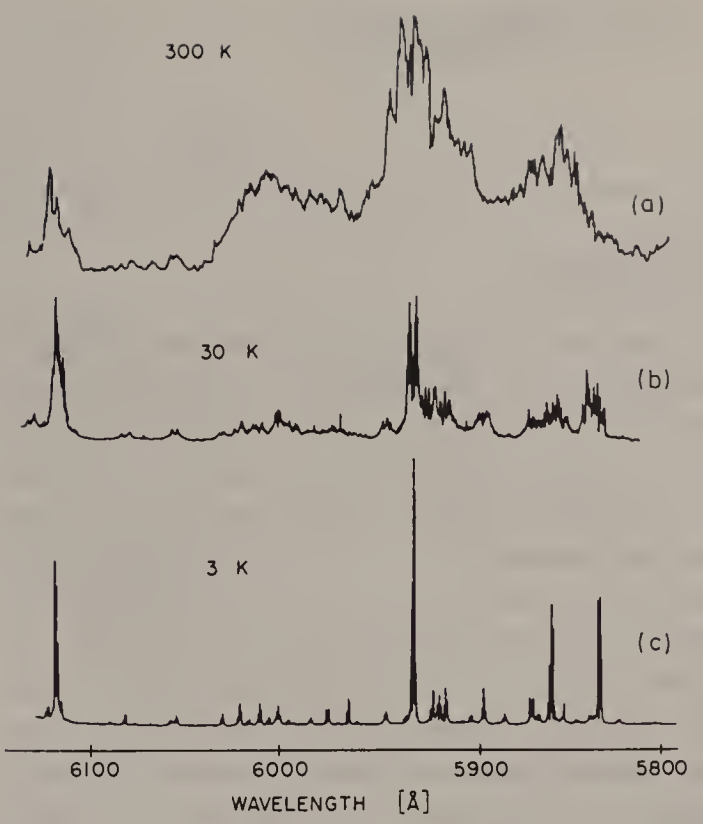


Fig. 1 Example in the reduction in congestion of the luminescence spectrum of a small polyatomic molecule (NO_2) produced by placing the molecule of interest in a supersonic expansion. (a) Room temperature sample of NO_2 (b) supersonic beam of pure NO_2 (c) supersonic beam of NO_2 highly diluted in argon. (D.H. Levy, L. Wharton, R.E. Smalley: Laser Spectroscopy in Supersonic Jets, in *Chemical and Biochemical Applications of Lasers*, Vol. 11 (ed. C. B. Moore). Academic Press, New York, 1977).

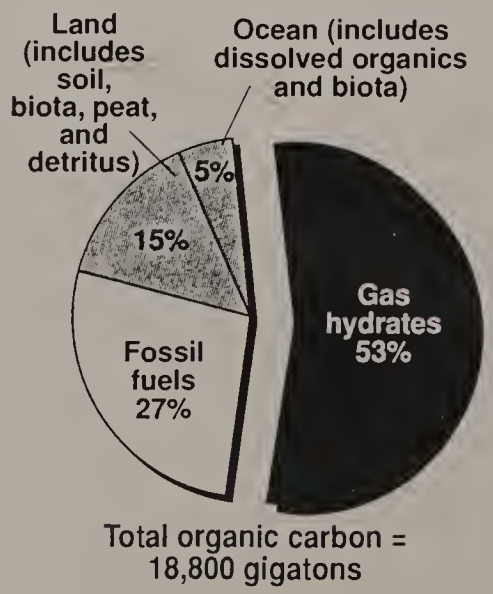
Inhomogeneous broadening of the homogeneous linewidth occurs when the molecule of interest is strongly coupled to its surroundings. For example, absorption/emission spectra of guest molecules in solid host matrices are inhomogeneously broadened and their linewidth can be, of order, 100–300 cm^{-1}. The homogeneous linewidth may be smaller than the inhomogeneous bandwidth by several orders of magnitude. These broadened bands are formed from homogeneous lines densely distributed over a large spectral range. This distribution results from the interaction of the probe molecule's potential surface with the different molecular microenvironments present in the host matrix. To a good approximation, the inhomogeneous band profile can be described by a Gaussian function, whereas the homogeneous line shape has a Lorentzian profile. A Gaussian distribution of Lorentzian lines produces a Voigt profile.

News

Gas hydrates

One of the many things for which Michael Faraday is remembered is an investigation of the pressure and temperature dependence of the solubility of simple gases in water. He discovered, what we now call, clathrates. These materials, which are normally formed at low temperature, close to 0 °C, and moderately high applied gas pressure, arise because certain gas molecules are just the appropriate size to be trapped into the open structure of the solid formed when the water freezes. Ice has an open structure held together by hydrogen bonds, the empty cavities present in the ice structure can accommodate small molecules, for example, methane, ethane, chlorine and hydrogen sulfide. However, if the molecules of the gas are too large for the ice structure, then no clathrate will form. Likewise, if the molecule is too small, helium or neon, it will simply diffuse out from the solid ice leaving behind pure frozen water.

Methane, natural gas, forms a clathrate at temperatures below 20 °C and at pressures of methane in excess of 20 bar. Thus, in any situation where water and methane are found in contact, under the above physical conditions, a clathrate will form. This happens in the laboratory and in the oil-field. The methane clathrate is a crystalline solid which has been responsible for blocking valves in many of the pipelines which transport natural gas across Arctic landscapes, for example, Alaska, when the natural gas has not been sufficiently dried at the well-head.



Note: Estimated distribution of organic carbon in Earth reservoirs (excluding dispersed carbon in rocks and sediments, which equals nearly 1,000 times this total amount). Atmospheric carbon estimated to be 3.6 gigatons.
Source: U.S. Geological Survey

Gas hydrates hold huge reserves of organic carbon.

It was recently reported at a meeting of the American Association for the Advancement of Science in Atlanta that global deposits of methane clathrate are estimated to contain twice as much carbon as all other fossil fuels on Earth. It was shown that the conditions necessary for the formation of these clathrates are met beneath the ocean floor on continental margins and in regions north of the Arctic Circle.

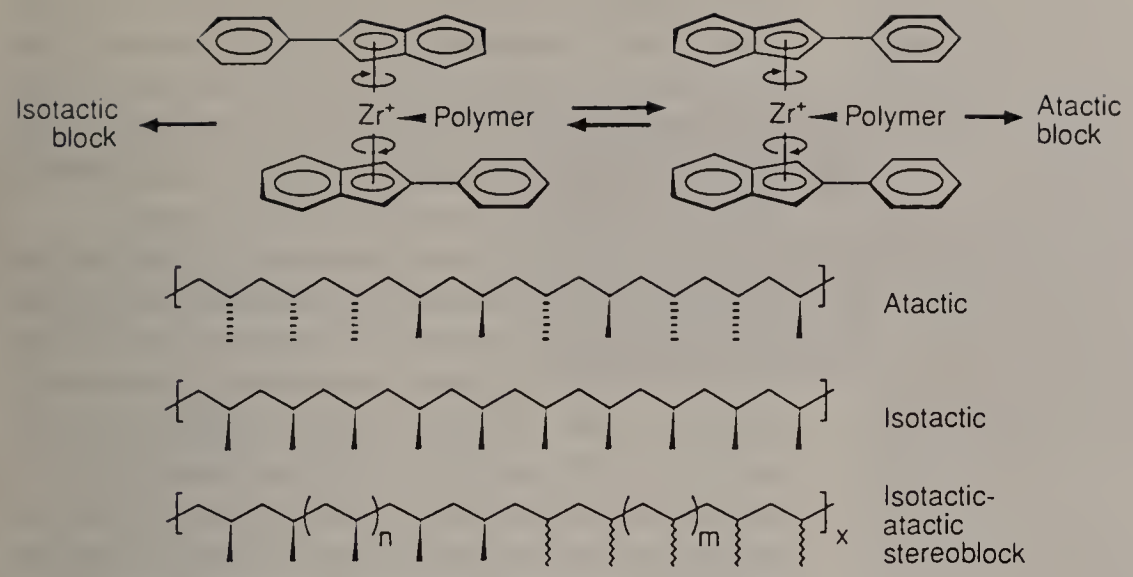
Unfortunately, methane hydrate is a solid and consequently not amenable to conventional gas recovery technology. However, engineers at the meeting in Atlanta identified two potential recovery techniques for gas hydrates. One involves injecting a warmer fluid, e.g. sea water, into the hydrate deposits which will then dissociate allowing a conventional recovery of the liberated methane. Another technique involved reducing the pressure applied to the hydrate deposit, perhaps by drilling into the deposits, thereby causing its dissociation and subsequent harvesting. After discussion, it was thought that drilling to induce a pressure reduction would probably be the best approach for methane recovery. However, it was not clear as to the best way to go about such drilling. The environmental effects of such drilling are, at present, uncertain. Methane is a greenhouse gas and any large-scale release of methane into the atmosphere could affect the Earth's climate. Methane release from deposits is believed to occur naturally, however, large-scale drilling could significantly increase the amount of gas entering the atmosphere.

The figure shows how important these reserves of methane hydrate could be to our future energy needs. At present, there is still much uncertainty as to the best technique for recuperating the methane, and the cost of readily available methane is low, however, it is a natural resource which will not go away and will be available when our technology improves.

Oscillating catalysts

Polypropylene is one of the most common of modern polymers, it is among the five largest volume plastics in the world, with millions of tons produced each year. It is found in electrical appliances, bottles, carpets, clothing, drinking glasses, everywhere. However, it is one of the newer plastics, a product of the 1950s work of Ziegler and Natta. The raw material for this polymer is propylene, a cheap oil-derived gas.

Ziegler and Natta won the 1963 Nobel prize in chemistry for their work in stereoregular polypropylene, that



Oscillating catalyst produces stereoblock polymers

is, attempting to understand the stereochemistry of the polymerization of propylene. Stereoregularity is the key to useful applications of the polymer material because it leads to mechanical strength and ease of processing. The stereoregularity of the polymer can be defined in terms of its tacticity. For example, if all the stereocenters in the polymer are the same, then it is said to be isotactic. If the stereocenters alternate back and forth in their identity, then the polymer is syndiotactic. If there is no control of the stereochemical placement, then the final polymer is atactic.

Isotactic polypropylene in which all the stereocenters in the polymer are the same is a crystalline thermoplastic. By comparison, atactic polypropylene, in which the stereocenters are randomly arranged is an amorphous gum elastomer. Bulk polypropylene consisting of blocks of atactic and isotactic stereosequences is rubbery. Consequently, the manner of polymerization strongly determines the characteristic of the final polymer. The polymerization reaction begins with a fixed chiral center found within the catalyst itself, and this center initiates a chain reaction of tens of thousands of monomer molecules to produce the polymer. The reaction is fast, with each new propylene molecules being inserted into the growing polymer chain one at a time. The extraordinary aspect of the Ziegler-Natta chemistry is that each insertion of propylene occurs with nearly perfect stereochemical precision, thereby producing the same stereocenter each time.

G. W. Coates and R. M. Waymouth (Department of Chemistry, Stanford University, USA) have recently demonstrated (*Science*, **267**, 217 (1995)) a strategy for the synthesis of thermoplastic elastomeric polypropylene based on the catalytic activity of the unbridged metallocene bis(2-phenylindenyl) zirconium dichloride [$(2\text{-PhInd})_2ZrCl_2$]. This catalyst was designed to isomerize between achiral and chiral coordination geometries during the polymerization reaction to produce atactic-isotactic stereoblock polymers. The metallocene precursor $(2\text{-PhInd})ZrCl_2$, in the presence of methylaluminoxane, polymerizes propylene to yield rubbery polypropylene. The isotacticity of the polymer, described by the isotactic pentad content (the fraction of stereosequence containing five adjacent isotactic stereocenters), increases with increasing propylene pressure and decreasing polymerization temperature to produce polypropylenes with an isotactic pentad content ranging from 6.3–28.1%.

The Stanford chemists built on the work of others who showed that rigid, chiral metallocene catalysts produced isotactic polypropylene, whereas achiral forms of the catalyst produced atactic polypropylene. The Stanford group therefore prepared an unbridged metallocene catalyst with indenyl ligands that rotate about the metal-ligand bond axis. This rotation causes the catalyst to oscillate between chiral and achiral geometries. When in a chiral position, it synthesizes a block of isotactic polypropylene; when in an achiral position it synthesizes a block of atactic polypropylene. As the ligands oscillate between these two positions, an oscillation which is strongly temperature dependent, alternating blocks of atactic and isotactic polymer are produced.

The figure shows the mechanism of polymerization for this new catalyst and the arrangements of the stereocenters in the different types of polymer material. This new catalyst allows chemists to control the mechanic properties of the polypropylene over a wide range. New materials may be produced which can be stretched to eight times its length and snaps back, or materials can be manufactured which are stiff and hard.

The weakest chemical bond

The element argon is named for its chemical innertness – *argos* being Greek for inactive. Indeed, it is one of a group of elements known as the inert gases. The fact that all of these elements are gases is a measure of

their lack of chemical reactivity – they do not want to form bonds with anything. These elements have closed electronic configurations and it requires considerable energy to break this stable arrangements of electrons to allow participation in chemical bonding.

Eventually, theoretical examination of the ionization potentials of these inert gases revealed that it could be possible to form compounds involving some of the more easily ionized gases with extremely powerful oxidizing agents. These materials were subsequently prepared, and the chemists involved won a Nobel prize. However, compounds consisting of only inert gas elements do not exist under normal laboratory conditions.

When one closed-shell atom approaches another closed-shell atom, e.g. argon–argon, a long-range attractive potential develops between them. This force arises because instantaneous fluctuations in the charge distribution on one atom correlate with similar fluctuations on the other atom, resulting in an attractive dispersion interaction which operates with an R^{-6} distance dependence. This interaction, is a manifestation of a departure from the ideal behaviour for these gases and is termed a van der Waals interaction.

As the two atoms approach one another under the influence of this attractive force, they will eventually arrive at a certain distance where their charge distributions begin to repel one another – a short-range repulsion. The balance between these attractive and repulsive forces gives an energy minimum, and in two dimensions has the familiar form, for example, as a Lennard–Jones 6–12 potential. For two argon atoms, the energy minimum, the bond strength of the dimmer, is very weak. Indeed, this bond energy is less that the energy available in thermal fluctuations at normal temperatures. So when another argon atom collides with an argon dimmer at laboratory temperatures, the collision transfers sufficient energy to break the weak van der Waals bond between the two argon atoms in the dimmer.

If the bond energy between two argon atoms is small, of order, 200 K, that between two helium atoms will be very much smaller. The dispersion interaction scales as the square of the electronic polarizability (α) of the two atoms (α^2_{argon}), which itself scales as the volume of the atom ($\alpha_{argon} \approx$ volume of argon atom). Recently however, Prof. Ronald Gentry, University of Minnesota, USA, has succeeded in producing helium dimmers and, for the first time, measuring the length of the very weak bond between two helium atoms in a dimmer.

Gentry *et al.* produced their helium dimmers in the collision free environment of a molecular beam. Here adiabatic expansion of a gas through a small hole, from a high pressure zone into a vacuum, causes a condensation of the atoms into small clusters. To measure the bond length of the dimmers present in their molecular beam, the scientists shot their molecular beam at a series of sieves with a series of holes just a few hundred nanometers in diameter. The larger a molecule, the more likely it is not to pass through a hole, by varying the size of the hole and counting the number of molecules which pass a particular sieve, the scientists could determine the size of the helium dimmer.

Amazingly, Gentry *et al.* discovered that the helium atoms were on average 62 Å apart, making it by far the longest diatomic molecule. To interpret such a long bond, the authors invoke Heisenberg's uncertainty principle. Since the atoms in the 'molecule' are very slow moving, they are close to the absolute zero of temperature, the uncertainty in their momentum will be small. Thus the uncertainty in their position must, by virtue of Heisenberg's principle, be large. Indeed, calculations suggest that the helium-helium bonds are not uniformly 62 Å apart, but vary in separation between 3 and 100 Å – very floppy molecules.

Advances in light-emitting devices

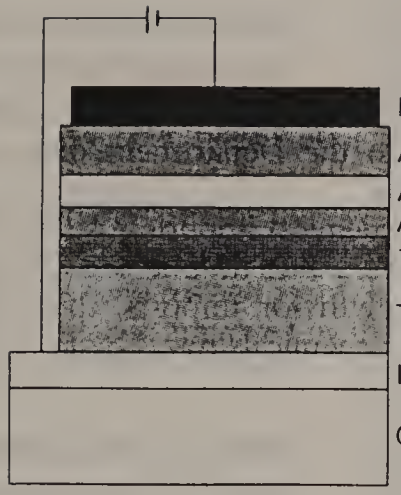
New reports show how scientists are making steady progress in the fabrication of organic devices which emit white light.

The latest such device comes from Japan, where researchers have found a way of creating a light-emitting diode (LED) which glows nearly as brightly as a fluorescent tube. The device is shown in the accompanying figure and can be seen to be a layered structure which is subjected to an applied potential. The researchers have developed a system where the different organic layers emit light of different wavelengths, blue, green and red, and the net result of the overall emission being white light.

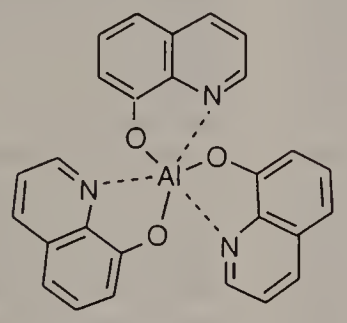
The light is produced by the recombination of holes (positive charges) and electrons injected into the organic material from the electrodes at opposite ends of the sample. The reaction of radical cations, molecules which have lost an electron (holes) and radical anions, electron-rich species, produces molecules in excited states which emit light of a characteristic wavelength as part of its decay process.

This work, reported in *Science* (**267**, 1332 (1995)), is from the laboratory of materials scientists J. Kido, M. Kimura and K. Nagai of Yamagata University, Japan.

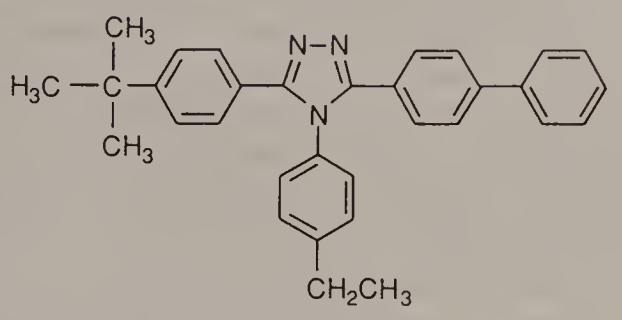
In the last couple of years a number of research groups have reported multilayer organic structures which produce white light. The Yamagata group has been one of the main players in these developments, last year they reported a device made from polymeric material doped with three different types of fluorescent dyes, each doped material emitting light of different wavelength – blue, green or red, to produce white light. Now the group has combined this doping approach with the design of a structure containing three different chemically distinct types of emitting layer.


Magnesium-silver contact (injects electrons)
Alq (transports electrons; does not emit light)
Alq doped with Nile Red (emits green + red = yellow light)
Alq (emits green light)
1,2,4-Triazole derivative (transports electrons, blocks holes)
Triphenyldiamine derivative (emits blue light)
Indium-tin oxide contact (injects holes)
Glass substrate

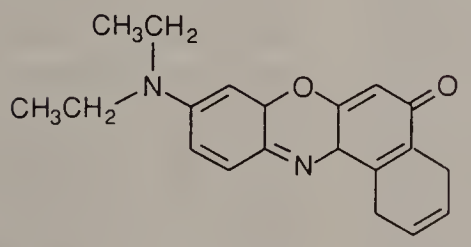
Device's organic layers emit three colours of light.



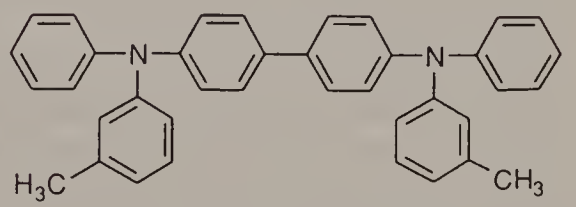
8-Hydroxyquinoline aluminum complex (Alq)



1,2,4-Triazole derivative



Nile Red



Triphenyldiamine derivative

The Japanese group report that their three layer device achieves a maximum luminescence of 2200 candela per square meter (cd/m^2) at a relatively low applied voltage of 16 V. By comparison, a cathode ray tube monitor puts out about 100 cd/m^2, and standard fluorescent lamp about 8000 cd/m^2.

Kido hopes to develop battery operated flat-top full-colour displays by using a white light-emitting device combined with micropatterned colour filters. Such a device would not use a liquid crystal layer, so the device would be inherently more efficient with a faster response time than a current LCD system.

IUPAC activities in environmental chemistry

It is probably true to say that we are all concerned about the quality of the environment. Irrespective of which country we live in, we are all confronted in our daily lives by evidence of the mismanagement of the environment. The Rio Earth Summit in 1992 was an unprecedented response by our governments to the problems raised by pollution and global warming. The governments recognized that it is not a problem for one or a few national governments, but has implications for us all.

IUPAC is the international body of chemists, and as such has the potential for making immense contributions to the fight against continuing degradation of the environment. Indeed, a recent survey of the Union's current activities in environmental chemistry has revealed a considerable effort being directed to this area in many branches of chemistry. At the 64th IUPAC Bureau meeting in Lisbon, 1993, Prof. Jack Calvert (Co-ordinator for Environmental Chemistry Activities in IUPAC and Senior Research Associate, National Center for Atmospheric Research Boulder, CO, USA) was asked to determine exactly the amount of IUPAC work devoted to identifying and attempting to solve problems in environmental chemistry.

It was observed that the number of studies related to environmental chemistry within IUPAC is truly impressive. The degree of activity within the various Divisions may be readily judged from the number of articles, related to environmental chemistry, recently published in official IUPAC journals and reports: Physical Chemistry Division(I) 41, Inorganic Chemistry Division (II) 19, Or-

ganic Chemistry Division (III) 19, Macromolecular Division (IV) 5, Analytical Chemistry Division (V) 113, Applied Chemistry Division (VI) 117, Clinical Chemistry Division (VII) 20, Committee on Chemistry and Industry (COCI) 2 and CHEMRAWN Committee 2. Due to the nature of the work, it is not surprising that the majority of these relevant reports come from the Analytical and Applied Divisions.

The subject mater of these investigations range from *Air chemistry* (trace gas analysis) to *Analysis of soil residues*, taking in, *Analysis of ground water* and *Analysis of foods for inorganic and organic contaminants*. With this great number of environmentally relevant projects it may be that there will be some overlap of activities, however, it is likely that although the areas of investigation are similar, the subject matter is being investigated from widely different perspectives and with different techniques. Environmental chemistry is a cross-disciplinary subject where the expert scientists are likely to have trained in a wide variety of field in chemistry and physics before becoming environmental chemists. IUPAC contains such a heterogeneous mixture of different chemists and, consequently, IUPAC environmental chemistry projects are likely to be some of the most thorough in their perception of the problem and their suggestions for solutions.

A good example of a useful IUPAC publication is *Gas Kinetic Data Evaluation for Atmospheric Chemistry* produced by the Physical Chemistry Division. This compilation continues a series, on rate and photochemical data, which are internationally recognized for their usefulness in modelling and understanding atmospheric chemistry. IUPAC publications related to evaluations of specific properties of trace impurities in the atmosphere, lithosphere or the hydrosphere are required in many environmental studies. 'Best values' for rate constants, solubility data, Henry's Law coefficients, optical cross-sections in a variety of wavelength regions, etc., are essential as input for good modelling studies.

The need to protect the environment is not solely the problem of the industrialized nations. There is a shortage of well-trained environmental scientists in the developing world, a shortage which will be aggravated with economic growth in those countries. It is to assist in training of chemists from developing countries who are aware of the importance of preserving the natural environment that IUPAC has set up, with UNESCO and UNIDO a joint training program in safety and environmental protection in chemical, pharmaceutical and biotechnological research and production. The training program was established in 1993 following two successful IUPAC Workshops on Safety in Chemical Production. The program is continuing with safety experts from Argentina, Bulgaria, China, Nigeria, etc., receiving in-depth training at IUPAC Company Associates.

The CHEMRAWN Committee continues to provide a useful forum for the international discussion of areas of concern related to environmental chemistry. The recommendations of international experts which arise from the CHEMRAWN activities should be an important input to decision makers and politicians.

Prof. Jack Calvert's document, Review of Activities Related to Environmental Chemistry Within IUPAC, *has been well received within IUPAC, and circulated to interested international agencies.*

Production of the Top 20 Chemicals in the US Increases Substantially in 1994

Rank			Billions of kg	
'94	'93		'94	'93
1	1	Sulfuric acid	47.2	41.6
2	2	Nitrogen	35.7	30.4
3	3	Oxygen	26.3	23.9
4	4	Ethylene	25.7	21.8
5	5	Lime	20.3	19.7
6	6	Ammonia	20.1	17.8
7	10	Propylene	15.3	11.8
8	7	NaOH	13.7	13.2
9	9	Phosphoric acid	13.4	12.2
10	8	Chlorine	12.8	12.6
11	11	Na_2CO_3	10.9	10.5
12	12	$C_2H_2Cl_2$	9.9	9.5
13	15	Nitric acid	9.4	8.7
14	14	NH_4NO_3	9.3	8.7
15	13	Urea	8.5	8.8
16	17	Vinyl chloride	7.8	7.3
17	16	Benzene	7.8	7.4
18	18	Methyl *t*-butyl ether	7.2	6.8
19	20	Ethylbenzene	6.3	6.3
20	22	Styrene	6.0	5.3

Production in the United States of the 20 largest volume chemicals reached a record level in 1994, following a modest increase in 1993. However, chemical industry analysts and economists say that this increase in growth is unsustainable, and 1995 growth will be weaker.

The US experienced stronger than expected domestic economic expansion. The Chemical Manufacturers Association pointed out that economists had to revise their estimates of growth from late 1993 to late 1994. The primary end use drivers for chemicals, that is, vehicles and housing, were particularly strong. There was strong growth, 14%, in the light-vehicle sector, with more than 15 million units sold last year with each unit requiring about USD2000 worth of chemical processing. Housing starts were also stronger than expected, up 13% to 1.5 million units, the highest level since 1988.

Chemicals destined for use in plastics showed particularly high growth in 1994. Petrochemicals were favorably priced, so that synthetics were able to take

market share from paper, cotton and other natural products. Ethylene production rose along with ethylene oxide and ethylene glycol. Ethylbenzene output was up a modest 0.9%, this is an intermediate for styrene (up 12%) manufacture, which is an intermediate for the production of polystyrene (up 3.1%). Caprolactam, production up 24%, is a derivative of phenol and is used in the production of nylon (up 3.3%). Cumene, for which production was up 15%, accounts for about a quarter of benzene end use, is used in phenol and phenolic resins production (production up 4.2%).

Sulfuric acid remains, as it has done for more than two centuries, the largest volume manufactured chemical. Roughly two-thirds of the demand for sulfuric acid is for fertilizers. Nitrogen maintained its number two position. The strong areas of nitrogen's diverse uses in industry include petrochemicals, metallurgy and electronics – all of which continue to grow.

Synthetic polymers – plastics, synthetic fibers and synthetic rubbers – all sustained robust growth in 1994. Increasing substitution of these materials for paper, natural fibers and natural rubber, together with a growing economy, lead to an overall increase in output of 7.2% over 1993. Plastics which account for more than three-quarters of total polymer production grew by 7%.

Growing employment income in the US, and increasing economic optimizm stimulated demand for nondurable goods such as packaging, which represents 41% of resin end use. Combined with low interest rates, the year recorded strong growth for durable goods – a good market for chemicals.

Housing starts in the US were up – building and construction account for 20% of resin sales. Polyvinyl chloride contributed about 68% of its output to the construction industry. For example, sales of PVC piping rose by 10% in 1994, high-density polyethylene pipe sales rose by 15%, helping to lift US production of high-density polyethylene to almost 6 billion kilos.

Other areas where plastics are replacing natural products include high-density polyethylene plastic grocery bags, output up 17% over 1993. Production of plastic food bottles, the largest single end use for high-density polyethylene, grew by 5% to 0.7 billion kilos.

Noncellulosic fibers production grew 7.5% to 5 billion kilos. They were affected slightly by environmental concerns. Noncellulosic fibers are much in demand because they are easy to produce and process. Olefin and nylon fiber also benefited from growth in automobile production and housing starts, which propel, for example, an increased demand for carpeting. However, it was the production of synthetic rubber which gave the best showing interms of increased demand, up 10%. This increase was driven primarily by the boost in the automobile industry – tires are the end use of 84% of solid styrene-butadiene and 76% of polybutadiene in the US.

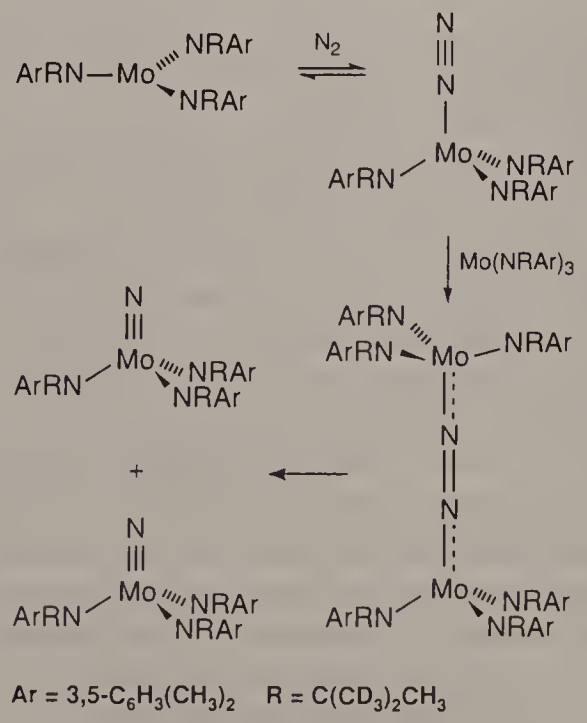
Fixing nitrogen

Chemists have had a fixation about nitrogen fixation for almost a century. Biologists recognized that biological systems could fix nitrogen to produce the materials needed for life. However, chemists were a little slower in showing how they could fix nitrogen. It was not until 1913 that Fritz Haber and the BASF (*Badische Anilin und Soda-Fabrik*) chemist Carl Bosch showed that an iron catalyst could be used to fix atmospheric nitrogen into ammonia. This Haber-Bosch nitrogen fixation proved to be essential in helping Imperial Germany meet its agricultural and military needs when the British Royal Navy blockaded European ports during the First World War.

Although the Haber-Bosch process has been much studied and the conditions necessary for operation maximized and fine tuned, there is as yet no detailed understanding of the mechanism of his fixation process. However, it is likely that the rate determining step is the breaking of the N≡N triple bond.

Detailed work on the biological mechanism of nitrogen fixation started with the isolation of cell-free extracts of nitrogenase in 1960. Chemists became interested in the problem when Vol'pin described the reaction of highly reduced metal salts with N_2 in 1964. The focus of much chemical work since the results of Vol'pin has been to understand how one or two metal atoms can supply the six electrons required to convert N_2 to two N^{3-} ions and also to supply an environment suitable for the stabilization of these nitrides. This scenario is less of a problem in nitrogenase, because there is a continuing flux of protons and electrons to operate the cycle.

Over the last thirty years many dinitrogen complexes have been prepared. The first contains N_2 bonded end-



Molybdenum-nitrogen triple bond formation drives bond breaking

on to a metal atom – the bond within the bonded N_2 moiety being much the same as in free N_2. The second class of complexes contains N_2 bonded end-on to two metal atoms. The third class of complexes contain N_2 bridging two metal atoms, but with a N-N separation much greater than in free N_2 – see the table.

What is happening is that a system M ←N≡N→ M is moving towards M=N–N=M. The final stage would be M≡N N≡M. This final step is what has been achieved in a remarkably simple experiment by Laplaza and Cummins (*Science* **268** 861–863 (1995)).

A metal atom capable of splitting the N≡N bond should function both as a Lewis acid (electron acceptor), accepting electrons from the N_2, and should also supply electrons to weaken further, and eventually break the N≡N bond. The class of dinitrogen complexes with the long N–N bonds and the intermediates in the protonation of coordinated N_2 represent systems in which the N–N bond-breaking process has commenced, but in which it cannot continue without the introduction of additional reagents. An alternative would be to use two metal ions and require them to provide three electrons each, this is what Laplaza and Cummins have done with the Lewis acid $[\{(C_6H_3Me_2)Bu^tN\}_3Mo]$.

Compound N-N	Bond Length (Å)
N≡N	1.098
$[(NH_3)_3Os←N≡N]^{2+}$	1.12
$[(NH_3)_5Ru←N≡N→ Ru(NH_3)_5]^{4+}$	1.12
$[(N_2)(C_5Me_5)_2Zr←N=N→ Zr(C_5Me_5)_2(N_2)]$	1.182
$[((Et_2)NCS_2)_3Nb←N=N→ Nb(S_2CN(Et)_2)_3]$	1.252
Me–N=N–Me	1.25
$H_2N–NH_2$	1.454
$[\{(C_6H_3Me_2)Bu^tN\}_3Mo≡N]$	
$[N≡Mo\{NBu^t(C_6H_3Me_2)\}_3]$	No bond

Life has recently been busy in the MIT laboratory of Prof. Christopher Cummins. On 8 May 1995, *C&ENews* (Page 27) reported that a molybdenum complex prepared in Cummins' laboratory cleaves nitrogen-nitrogen bonds in N_2O. The reaction of a monomeric tris(amido) molybdenum (III) complex with nitrous oxide contrasts with previous such investigations, in that it is the N–N, rather than the N–O bond, of the nitrous oxide molecule which is cleaved. The molybdenum complex, $Mo(NRAr)_3$, where R is $C(CD_3)_2CH_3$ and Ar is 3,5-$C_6H_3(CH_3)_2$, was made to investigate redox reactions. The bulky side groups would inhibit dimerization, and subsequent X-ray crystallography has revealed that the molecule is a monomer, and magnetic measurements have revealed the presence of three unpaired spins. Exposure of the complex to NNO results in two products, $N≡Mo(NRAr)_3$ and $ON≡Mo(NRAr)_3$.

Such reactivity is surprising, because the N–N bond is stronger than the N–O bond in nitrous oxide.

Now, the 15 May 1995, *C&ENews* (Page 5) reports that the same laboratory has achieved the long sought after goal of directly cleaving, by a six electron reduction, dinitrogen in solution.

The initial experiments with the Mo complex showed its ability to undergo three electron reductions and not to dimerize. However, if two Mo complex molecules attach themselves to either end of a dinitrogen molecule, then a six electron reduction is possible.

Initially, the MIT group purified the red–orange Mo complex in diethyl ether under argon. However, when an atmosphere of nitrogen was substituted for the argon, the colour of the solution changed to deep purple. Deuterium NMR was used to investigate the purple species, and it was provisionally identified as a $(ArRN)_3Mo–N_2–Mo(NRAr)_3$ complex – see figure. Exposing a toluene solution of $Mo(NRAr)_3$ to dinitrogen produced the purple solution, which upon warming turned golden. Proton NMR showed that the species responsible for the golden colour was the product of the dinitrogen cleavage $N≡Mo(NRAr)_3$.

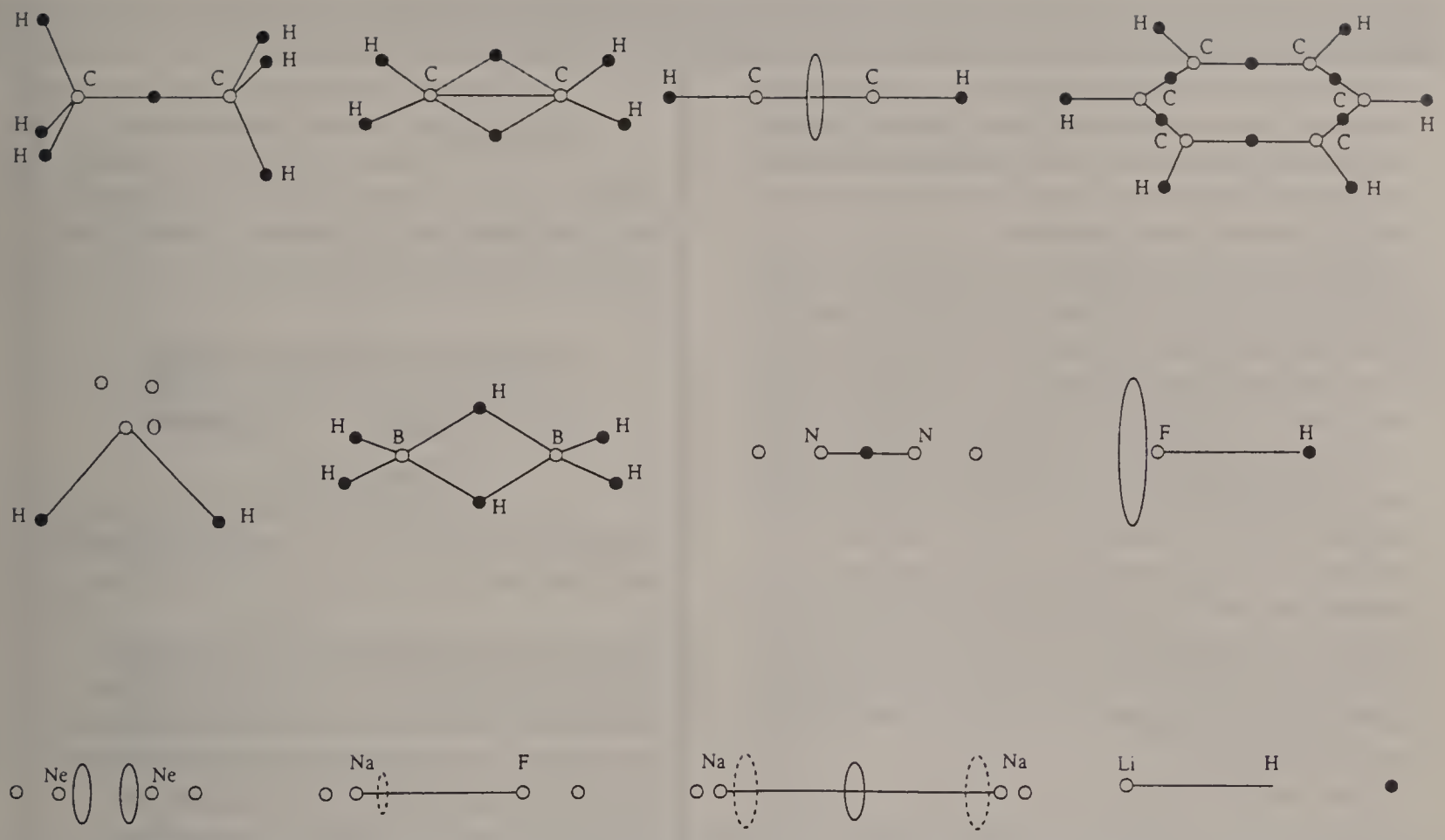
Given that Laplaza and Cummins' N_2 reduction duplicates the major step in the Haber–Bosch process, but at single metal atom sites rather than metal surfaces, the question arises as to the application of this type of chemical reaction to industrially useful processes. The problem of regenerating the Mo complex starting material would have to be solved, however, perhaps an electrochemical approach would be of use here.

A New Look at Chemical Bonds

One of the many great achievements of the late Linus Pauling was his experimental work on electron diffraction by gas-phase molecules. This work, together with his many profound theoretical insights, formed the basis of *The Nature of the Chemical Bond* (Cornel University Press, 1948), one of the great chemical texts. Pauling showed how non-ionic chemical bonding could be rationalized by considering the pairing of electrons, and in this way how the shapes of molecules could be visualized by taking account of the repulsion between these pairs of electrons. This pioneering theoretical work was later extended in that other classic text, *Valence* (OUP, 1961) by Charles Coulson.

What determines the form and type of a chemical bond is, however, still very much an open question. The ideas go back to the days before quantum mechanics, for example, to Gilbert Lewis (Pauling's mentor) in 1916. However, a fully rigourous description of bonding, based firmly in quantum mechanics would be desirable, particularly, if it could be made quantitative. For in this way, one could determine *ab initio* the bond order or the covalency vs. the ionicity of a bond.

One of the quantities used most widely in a description of the pairing of electrons is the electron density



Bonding diagrams of: (top row) C_2H_6, C_2H_4, C_2H_2 and C_6H_6: (middle row) H_20, B_2H_6, N_2 and HF; (bottom row)Ne_2, NaF, Na_2 and LiH. The core, bonding and non-bonding points are represented by white, black and grey dots, respectively. Core ring attractors are draw as dashed lines, valence attractors in solid lines. The conventional structure is given by solid lines joining the nuclei. In shared–electron interactions, involving hydrogen, e.g. C_2H_6, the bonding attractors are very near the protons, whereas for hydrides such as LiH, the localization of the attractor is not very reliable because the localization function is close to unity. C_2H_4 and B_2H_6 have very similar attractor patterns, giving support to the 'banana bond' representation of the bonding in these molecules. Triple bond attractors degenerate into ring attractors, see C_2H_2, butcorespond to a single point as in N_2. The bonding ring attractor of Na_2 is related to a single pair. The diagrams for Na_2 and NaF show how symmetry breaking with respect to the free ion splits the Na L-shell sphere attractor into a point and a ring. The diagram for the neon dimer corresponds to a repulsive interaction, the internuclear separation having been constrained to 0.1 nm.

and how this electron density varies as a function of distance, $\rho(r)$. This quantity may be calculated using quantum mechanical computations, but it is also an observable in X-ray scattering experiments – the X-rays are scattered from local fluctuations in the electronic charge density. Any map of the positions of atoms in a solid determined by X-ray scattering is also a map of electron density.

The most useful technique in the analysis of $\rho(r)$ is to consider the electron density of the molecule or crystal being split into ever smaller fragments, or segments, and the way the density varies from one fragment or segment of the molecule to another. This method involves finding the steepest downhill paths through the electron density, that is, finding that part of the density which is changing most rapidly – maximum derivative of $\rho(r)$, i.e. $\nabla\rho(r)$. However, before determining the derivative of the charge density, one must first have a surface representing the molecule and the electron density between the atoms. This map of the electronic structure may be calculated, by large *ab initio* quantum mechanical calculations, or inferred from X-ray scattering experiments.

An alternative approach to the analysis of these electronic topologies, or electronic surfaces, is based on considering the ways in which the shapes or topological types of the three-dimensional contours (just like a survey map with contours of constant altitude represent lines of constant electron density) of the density map change at various maxima and minima on the surface. In this way, features on these surfaces which correspond to bonds may be identified. However, heavy, multi-electron atoms stand out clearly as large concentration of electron density and the bonds between such features are not so obvious. It is often difficult to discriminate between large features, the atoms, and minor features, the covalent bonds.

However, a new approach for unravelling and interpreting the maxima and minima on multi-dimensional electronic surfaces for molecules has recently appeared. This new approach of B. Silvi and A. Savin (Université Pierre et Marie Curie, Paris) has been published (*Nature* **371**, 683–686 (1994)) involves the use of an electron localization function which is a measure

of the influence of the Pauli exclusion principle on the local kinetic energy of an assembly of electrons. This is a relatively simple function of the electron density and the rate of change of this density; and unlike the previously used system of analysis this function takes values between zero and unity only. In this way it is a more clear cut method of interpretation.

The excess kinetic energy is found to take low values in regions occupied by paired electrons; this leads to values of the electron localization function close to unity. Silvi and Savin then map out the location of all modulations of the electron localization function on the electron density map of a molecule and are able to deduce much about the chemical bonding present in the molecule under investigation. For the molecules that they consider, the locations of the electronic core, bonding and non-bonding electrons appear to be consistent with conventional representations of the electronic structure. That is, the theoretical interpretation agrees with what a chemist knows about the bonding in these molecules.

In the absence of symmetry in the system, the Pauli principle implies saturation at two electrons per point of localization in the molecule, the authors call these points 'attractors'. Integrating $\rho(r)$ over these points of localization (attractors) provides information on the degree of saturation and on the bond multiplicity.

Silvi and Savin have provided the first step in the development of an exciting new non-empirical approach to the classification of chemical bonding. Their method seems to work well for small closed shell molecules (see figure), however, the test will come when it is applied to more controversial cases, for example, FOOF the fluorinated analogue of hydrogen peroxide.

Names and addresses

Full details (names, addresses, telephone/telex/Fax: numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* **15** 215–227 (1993). The IUPAC Secretariat have been notified of the following changes:

Prof. Dr Ekkehard Fluck, E-mail: fluck@mpigm-frankfurt.mpg.d400.de

Prof. Albert Fischli, E-mail: albert_e.fischli@roche.com

Prof. K. I. Zamaraev, State Research Center Boreskov, Institute of Catalysis, 5 Prospekt Akademika Lavryentyeva, RU-630090 Novosibirsk 90, Russia.

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ICOS 11
30 June – 4 July, 1996
Amsterdam, the Netherlands

Thieme Publishers and IUPAC in collaboration with the editors of *Synthesis*, *Synlett* and *Houben-Weyl* announce the 1996

Thieme–IUPAC Prize in Synthetic Organic Chemistry

sponsored by Georg Thieme Verlag of Stuttgart and New York.

The Thieme–IUPAC Prize is presented every two years on the occasion of the International Union of Pure and Applied Chemistry – International Conference on Organic Synthesis (IUPAC–ICOS). The 1996 ICOS will be held in Amsterdam, the Netherlands, on June 30 – 4 July.

Prize DM 10 000

The prize is awarded to a scientist under 40 years of age (as of 1 January of the year in which the prize is awarded) whose research has had a major impact in synthetic organic chemistry.

The first Thieme–IUPAC Prize was awarded in 1992 to Stuart L. Schreiber (Harvard) and the second in 1994 to Paul Knochel (Marburg).

Call for Nominations (deadline December 15, 1995)

The prize will be awarded on the basis of scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials. Proposals must be accompanied by a biographical sketch of the nominee, a list of the candidate's 10 most significant publications, and a statement of how the candidate's research has had a major impact on the field of synthetic organic chemistry.

Nomination materials (8 copies) should be submitted by 15 December 1995 to the IUPAC Information Officer, IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK. Telephone +44 (1865) 747744. Fax +44 (1865) 747510.

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THE GORDON AND BREACH PUBLISHING GROUP

Publications

Solubility Data Series, Volumes 58 and 59 Polycyclic Aromatic Hydrocarbons: Binary Non-Aqueous Systems. Part I: Solutes A–E, Part II: Solutes F–Z

These two volumes complement Volume 54 of the Solubility Data Series, Polycyclic Aromatic Hydrocarbons in Pure and Binary Solvents. The two present volumes contain solubility data collected from the literature published up to mid-1994 for acenaphthene, anthracene, benzo[ghi]perylene, biphenyl, carbazole, coronene, fluorene, fullerene (C_{60}), naphthalene, phenanthrene, pyrene, thianthrene and other two- through six-ring polycyclic aromatic hydrocarbons dissolved in single non-aqueous solvents. Also included are any solubility data published from 1992 to mid-1994 for binary solvent systems after the completion of Volume 54. Data for well over 400 different systems were retrieved. The experimental values have been evaluated critically using standard statistical and thermodynamic methods. For polycyclic aromatic hydrocarbons dissolved in mixtures of two solvents, critical evaluations use predictive equations derived from Mobile Order Theory and the Combined Nearly Ideal Binary Solvent (NIBS)/Redlich–Kister Model. These predictive methods are of great value in the absence of confiratory data from more than one laboratory, a situation that is common for most of the studies on these systems. They facilitate interpolation between measured data points and aid in screening experimental data sets for possible outliers (incorrect values) which require redetermination.

The Solubility Data Series has been published as a journal since 1994, and a discount of 25% for both a subscription (four issues) and individual volumes applies to all IUPAC member, including members of IUPAC Commissions and Committees, and Affiliates.

The price to IUPAC members for a subscription is GBP199/USD296 (compared to the full price of GBP265/USD395). For individual volumes, IUPAC members may purchase these for GBP60/USD90 each (compared to the full price of GBP80/USD120). Please note that Sterling rates apply in UK and Europe, United States Dollar rates apply elsewhere.

Polycyclic Aromatic Compounds: Binary Non-aqueous Systems, *Part I:* Solutes A–E*; Part II:* Solutes F–Z *(Volumes 58 and 59 of the Solubility Data Series) were edited by W. E. Acree, Jr. and published by Oxford University Press, Walton Street, Oxford OX2 6DP, UK (Tel.: + 44 1865267907). 1995; xlv + 337 pp. ISSN 0191-5622.*

Molten Salts Bulletin '*Sels Fondus*'

The latest bulletin, 1995 No.56, in this series has been produced and contains a recent bibliography and details of recent conferences devoted to the study of molten salts. To continue this series of publications, interested readers are requested to send information and reprints concerning their work in this field to:

Molten Salts Bulletin Sels Fondus, M. Gaune-Escard, Institut Universitaire des Systèmes Thermiques Industriels, UA 1168, Université de Provence, Centre St. Jérôme, 13397 Marseille Cedex 20, France.

Thermodynamics of Enzyme-Catalyzed Reactions: Part 3. Hydrolases

This substantial review is a continuation of the first two papers in this series (*J. Phys. Chem. Ref. Data* **22**, 515 (1993) and **23**, 547 (1994)) that deal, respectively, with the thermodynamics of the reactions catalyzed by the oxidoreductases and by the transferases. These were the first two classes of enzymes classified by the Nomenclature Committee of the International Union of Biochemistry.

Reactions of hydrolases play significant roles in metabolic processes such as glycolysis, oxidative phosphorelation, glycogen and starch utilization, in the action of muscles and in the synthesis of genetic material. There is also special interest in many reactions involving hydrolases due to their importance in the utilization of biomass and cellulosic materials.

The data presented in this volume is limited to equilibrium and calorimetric measurements performed on these reactions under *in vitro* conditions. The data is presented in the same format as in the earlier volumes and the following information is given for each entry: the reference for the data; the biochemical reaction studied; the name of the enzyme used and its Enzyme Commission number; the method of measurement; the conditions of measurement (temperature, pH, ionic strength, and the buffer(s) and co-factor(s) used); the data and an evaluation of it; and, sometimes, a commentary on the data and on any corrections which have been applied to the data or any calculations for which the data has been used.

Equilibrium constants are given as dimensionless quantities. However, the numerical value obtained for the equilibrium constant for an unsymmetrical reaction will depend upon the measure of composition and standard concentration selected for the reactants and products. Thus, for the chemical reaction

$$A_{(aq)} = B_{(aq)} + C_{(aq)}$$

$K_c = c(B)c(C)/\{c(A)c^0\}$, $K_m = m(B)m(C)/\{m(A)m^0\}$, and $K_x = x(B)x(C)/x(A)$. Here, c, m, and x are, respectively, concentration, molality, and mole fraction; $c^0 = 1$ mol $dm,^{-3}$ and $m^0 = 1$ mol $kg.^{-1}$ The equilibrium constant expressed in terms of mole fractions is automatically dimensionless. The symbols used in this compilation are given in a Glossary.

A subjective evaluation of the data is given in this review: A (high quality), B (good), C (average) and D (low quality). In making these assignments, the authors have considered the various experimental details which were provided in the different studies. These details include the number of measurements, the number of data points determined, and the extent to which the variable conditions of temperature, pH and ionic strength were investigated. A low rating is normally awarded when few details of the investigation under consideration were given. For example, in many of the papers cited, the major aim of the research was the isolation and purification of the enzyme as opposed to a detailed investigation of its kinetics. Thus, the equilibrium data was obtained as only the small part of the overall investigation.

A full description of the thermodynamics of biochemical reactions in physiological media would be beyond the scope of this review. However, the authors point out that their primary motivation is to provide some means for determining the position of equilibrium of the reactions under discussion. The apparent equilibrium constants given here can be conveniently used to calculate the extent of reaction under the stated set of conditions and are thus of use to engineers seeking to calculate the optimum conditions for the operation of a bioreactor. The enthalpy changes associated with these reactions are also important in determining the amounts of heating and cooling required to keep a bioreactor at its proper temperature.

For many biochemical reactions, the apparent equilibrium constant is a function of temperature, pH, pX and ionic strength. Thus, when performing Hess' Law and thermodynamic cycle calculations, it is necessary that the data for all of the reactions in such a calculation refer to the same set of conditions. However, for a reac-

tion where none of the reactants or products have ionizable groups or bind metal ions under the conditions of investigation, the thermodynamic quantities for the chemical reference reaction correspond directly to the transformed thermodynamic quantities for the overall biochemical reaction. For example, the biochemical hydrolysis of sucrose to D-glucose and D-fructose is:

$$\text{sucrose}_{(aq)} + H_2O_{(l)} = \text{D-glucose}_{(aq)} + \text{D-fructose}_{(aq)} \quad (1)$$

A chemical reference reaction involving specific species is:

$$\text{sucrose}^0_{(aq)} + H_2O_{(l)} = \text{D-glucose}^0_{(aq)} + \text{D-fructose}^0_{(aq)} \quad (2)$$

Here, the charges of the reference species have been specified to distinguish these moieties from the biochemical reactants. Since the extent of ionization of these sugars for pH < 10 is negligible, sucrose^0, D-glucose^0 and D-fructose^0 are the predominant species present in the reaction and the for pH < 10, $K'(1) = K(2)$, $\Delta_r H'^0(1) = \Delta_r H^0(2)$, and $\Delta_r G'^0(1) = \Delta_r G^0(2)$. Also, since $\Delta_r N(H^+) = 0$ for the second reaction, $\Delta_r H(cal) = \Delta_r H'^0(2)$. This situation is frequently encountered for the hydrolysis reactions of the disaccharides and oligosaccharides found in this review.

The work reported in this review has been accepted by the Thermodynamics Commission and by the Steering Committee on Biophysical Chemistry of IUPAC as a project of particular timeliness and importance. The document has been written to be consistent with recommended IUPAC nomenclature. It is hoped that this work will encourage additional efforts towards systematic data collection and evaluation for biochemical substances and reactions.

Thermodynamics of Enzyme-Catalyzed Reactions: Part 3. Hydrolases*; R. N. Goldberg and Y. B. Tewari, Biotechnology Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA. Published in* Journal of Physical and Chemical Reference Data*, **23**(6), 1035–1103 (1994).*

New Edition of *Surfactants Europa*

A revised and updated edition of the well-known directory *Surfactants Europa* will be published by the Royal Society of Chemistry in June, 1995. This directory will provide data on approximately 9000 trade names of surfactants manufactured and sold in Europe, by approximately 80 different manufacturers.

The directory is intended to provide easy access to up-to-date product information on European surfactant products, giving information on: surfactant type; supplier; trade name; properties and applications. The following information will, where possible, be included for each surfactant trade name: application, chemical class, chemical description, chemical name (CFTA name), cloud point, colour, composition, functionality, HLB number, ionic type, melting point, molecular weight, 'N' number, pH, physical characteristics, pour point, saponification number, supplier, surface properties, trade name and viscosity.

Surfactants Europa will also contain indexes of companies and trade names, and a manufacturers' address, including European divisions and agents. It is hoped that this directory will be a useful source of reference material for the laboratory as well as an essential document for the sales department.

For further details, please contact: Andrew Nightingale, The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF, UK. Surfactants Europa*, 3rd Edition (ISBN 085404 804 9), 450 pages, GBP 80.*

Modern Experiments for Introductory Chemistry

The Committee on the Teaching of Chemistry is grateful to the Division of Chemical Education of the American Chemical Society for permission to reprint a selection of articles from *Journal of Chemical Education*. The motivation behind this reprinting is to determine whether some of the more useful chemical education material published internationally can be made available to techers of chemistry in developing countries at a price which they can hopefully afford.

The experiments detailed in this volume cover a wide range of laboratory chemistry. For example, basic physico-chemical properties such as an estimation of Avogadro's Number using cetyl alcohol as a monolayer, to reaction kinetics such as the first-order decomposition of the violet coloured Ce(IV) oxidation product of *n*-phenylanthranic acid. There are also description of numerous experiments in both qualitative and quantitative analysis; for example, a thin-layer chromatography experiment for general chemistry, and the determination of copper in copper-nickel alloy, or the determination of the phosphoric acid content of cola beverages.

Reprinted from Journal of Chemical Education*, Modern Experiments for Introductory Chemistry, 2nd edition, Compiled by H. A. Neidig and W. J. Stratton; 135 pp., ISBN 0-910362-27-0, USD3.50 (paperback) and USD5.00 (hardback). Published by: Wiley Eastern Ltd, New Delhi 110 002 for IUPAC CTC and Printed at Presswork, 1813, Chandrawal Road, New Delhi 110 007. The IUPAC Committee on the Teaching of Chemistry and the publisher are granted distribution rights worldwide, except for the following areas: North American Free Trade Area, European Union, Japan,*

Australia and New Zealand. Sales may not be made, nor orders accepted from addresses within these areas. Sales of single copies are permitted at ICCE meetings to participants. Sales of single copies are permitted to individuals with addresses within Mexico, but not to corporations or booksellers. This is a specific exception to the North American Free Trade Area.

IUPAC Publications: 1975–1983

While many IUPAC titles from this period are no longer in print, this does not mean that they are no longer available. During its period as IUPAC's main official publisher, Pergamon Press published some 200 titles. Enquiries regarding these titles are now handled by Elsevier Science at the address given below.

Several of the first 53 volumes of the Solubility Data Series (1979–1992) may still be obtained from stock. Others may be obtained as single copies from the single-copy service provided by Franklin Books (Elkins Park, Pennsylvania, USA). They will provide you directly with a quotation for the supply of the title(s) of your choice. It is also possible to obtain, from Franklin Books, single copies of the 1979 edition of the *Nomenclature of Organic Chemistry*.

Stock of Solubility Data Series currently held by Elsevier (given in parentheses):

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- Cumulative Index: Volumes 1–18 (26);
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- Copper, Silver, Gold and Zinc, Cadmium. Mercury Oxides and Hydroxides (27);
- Propane, Butane and 2-Methylpropane (33);
- Metals in Mercury (34);
- Sulfites, Selenites and Telluritres (27);
- Methane (32);
- Mercury in Liquids, Compressed Gases, Molten Salts and Other Elements (49);
- Alkali Metal Halates, Ammonium Iodate and Iodic Acid (34);
- Alkali Metal Orthophosphates (34);
- Hydrogen Sulfide, Deuterium Sulfide and Hydrogen Selenide (11);
- Molten Alkali Metal Alkanoates (41);
- 4-Aminobenzenesulfonamides. Part I: Non-cyclic Substituents (26);
- 4-Aminobenzenesulfonamides. Part II: 5-Membered Heterocyclic Substituents (141);
- 4-Aminobenzenesulfonamides. Part III: 6-Membered Heterocyclic Substituents an Miscellaneous Systems (34);
- Hydrocarbons with Water and Seawater. Part I: Hydrocarbons C_5 to C_7 (0);
- Hydrocarbons with Water and Seawater. Part II: Hydrocarbons C_8 to C_{36} (0);
- Cumulative Index: Volumes 20–38 (156);
- Halides, Oxyhalides and Salts of Halogen Complexes of Titanium, Zirconium, Hafnium, Vanadium, Niobium and Tantalum (170);
- Alkaline Earth Metal Perchlorates (163);
- Hydrogen Halides in Nonaqueous Solvents (76);
- Carbon Monoxide (71);
- Copper and Silver Halates (161);
- Gases in Molten Salts (216);
- Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems) (171);
- Esters with Water. Part I: Esters 2-C to 6-C (233);
- Esters with Warer. Part II: Esters 7-C to 32-C (279);
- Carbon Dioxide in Non-aqueous Solvents at Pressures less than 700 kPa (196);
- Intermetallic Compounds in Mercury (199);
- Alkaline Earth Hydroxides in Water and Aqueous Solutions (184);
- Cumulative Index: Volumes 40–52 (0).

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Spanish Photochemistry

Glosario de terminos usados en fotoquimica – Spanish glossary of terms used in photochemistry – this is a translation into Spanish of the IUPAC document (*Pure & Appl. Chem.* **60**, 1055–1106) Glossary of terms used in photochemistry.

The translation has been undertaken by J. L. Bourdelande, S. Nonell, A. U. Acuna and R.Sastre with the collaboration of many Spanish, Portuguese and Latin American photochemists. A considerable effort has been made to find Spanish terms equivalent to those used in English. This glossary should be of use to all Spanish speaking photochemists. The translation was presented and approved at the 24th Reunion Bienal de al Real Sociedad Espanola de Quimica, and is published by Servei de Publicacions of the Universitat Autonoma de Barcelona (Apartado Postal 20, 08193 Bellaterra, Barcelona, Spain.

ISO Standards

April 1995

TC 27	**Solid mineral fuels**
ISO 540:1995	Solid mineral fuels – Determination of fusibility of ash – High-temperature tube method – Agricultural food products
ISO 688S:1995	Animal and vegetable fats and oils – Determination of conventional mass per volume (-litre weight in air-)
TC 47	**Chemistry**
ISO 9406:1995	Carbonaceous materials for the production of aluminium – Green coke – Determination of volatile matter content by gravimetric analysis
TC 172	**Optics and optical instruments**
ISO 11455:1995	Raw optical glass – Determination of birefringence
TC 176	**Quality management and quality assurance**
ISO 10013:1995	Guidelines for developing quality manuals
TC 183	**Copper, lead and zinc ores and concentrates**
ISO 11441:1995	Lead sulfide concentrates – Determination of lead content – Back titration of EDTA after precipitation of lead sulfate
TC 190	Soil quality
ISO 10694:1995	Soil quality- Determination of organic and total carbon after dry combustion (elementary analysis)
ISO 11261:1995	Soil quality – Determination of total nitrogen – Modified Kjeldahl method
ISO 11466:1995	Soil quality – Extraction of trace elements soluble in aqua regia

May 1995

TC 17	**Steel**
ISO 10278:1995	Steel – Determination of manganese content – Inductively coupled plasma atomic emission spectrometric method
TC 28	**Petroleum products and lubricants**
ISO 2176:1995	Petroleum products – Lubricating grease – Determination of dropping point
ISO 3648:1994**	Aviation fuels- Estimation of net specific energy
ISO 10370:1995**	Petroleum products – Determination of carbon residue – Micro method
TC 45	**Rubber and rubber products**
ISO 471:1995	Rubber-Temperatures, humidities and times for conditioning and testing
ISO 2454:1995	Rubber products- Determination of zinc content – EDTA titrimetric method
ISO 6235:1995	Rubber, raw – Determination of block polystyrene content- Ozonolysis method
ISO 8053:1995	Rubber and latex – Determination of copper content – Photometric method
TC 129	**Aluminium ores**
ISO 10277:1995	Aluminium ores – Experimental methods for checking the precision of sampling
TC 146	**Air quality**
ISO 7708:1995	Air quality – Particle size fraction definitions for health-related sampling
ISO 10155:1995	Stationary source emissions – Automated monitoring of mass concentrations of particles – Performance characteristics, test methods and specifications
TC 147	**Water quality**
ISO 10304–2: 1995	Water quality – Determination of dissolved anions by liquid chromatography of ions – Part 2: Determination of bromide, chloride, nitrate, nitrite, orthophosphate and sulfate in waste water
TC 190	**Soil quality**
ISO 10693:1995	Soil quality – Determination of carbonate content – Volumetric method
ISO 11048:1995	Soil quality – Determination of water-soluble and acid-soluble sulfate

June 1995

TC 28	**Petroleum products and lubricants**
ISO 9950:1995	Industrial quenching oils Determination of cooling characteristics – Nickel-alloy probe test method
TC 61	**Plastics**
ISO 4894–2: 1995	Plastics – Styrene/acrylonitrile (SAN) moulding and extrusion materials. Part 2: Preparation of test specimens and determination of properties
ISO 8988:1995	Plastics – Phenolic resins – Determination of hexamethylenetetramine content Kjeldahl method and perchloric acid method
ISO 9397:1995	Plastics – Phenolic resins – Determination of free-formaldehyde content – Hydroxylamine hydrochloride method
ISO 9771:1995	Plastics – Phenolic resins – Determination of the pseudo-adiabatic temperature rise of liquid resols when cured under acid conditions
TC 85	**Nuclear energy**
ISO 12183:1995	Controlled-potential coulometric assay of plutonium
TC 146	**Air quality**
ISO 10312:1995	Ambient air – Determination of asbestos fibres – Direct transfer transmission electron microscopy method
TC 174	**Jewellery**
ISO 11210:1995	Determination of platinum in platinum jewellery alloys – Gravimetric method after precipitation of diammonium hexachloroplatinate
ISO 11489:1995	Determination of platinum in platinum jewellery alloys – Gravimetric determination by reduction with mercury(I) chloride
ISO 11490:1995	Determination of palladium in palladium jewellery alloys – Gravimetric determination with dimethylglyoxime
TC 176	**Quality management and quality assurance**
ISO 10007:1995	Quality management – Guidelines for configuration management

Full details of these and other ISO Standards may be obtained from: ISO Central Secretariat, Case Postal 56, CH-1211 Geneva, Switzerland, Tel: +41 22 749 01 11, Fax: +41 22 733 34 30.

Conferences

VI International Congress on Automation and New Technology in the Clinical Laboratory (ANT),

XI International Congress on Computing in Clinical Laboratories (CCL), and

XIV Congreso Nacional de la Sociedad Española de Bioquímica Clínica y Patología Molecular; 2–4 November 1995, Sitges, Barcelona, Spain

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The scientific program of these meetings has been so arranged as to give a mixture of topics, which it is hoped will provide something for everybody. The scientific program will bring together the latest advances in clinical laboratory science. Researchers from around the world will gather to give talks and present papers on their research and exchange opinions on automation and computing in the clinical laboratory, as well as on theoretical and practical applications of the latest technological advances.

During the course of the conferences there will be a substantial exhibition displaying the most up-to-date laboratory equipment. Several companies will be using this meeting as a venu to launch new instruments.

The congress will consist of parallel plenary lectures and parallel symposia with associated poster sessions. For the ANT congress the symposia will be:

- Micro devices;
- Technology for sample handling;
- Impact of ISO9000 and other standards on the clinical laboratory;
- Advances in specific protein measurement;
- Automation in coagulation testing;
- Quality in the automated laboratory;
- New developments in particle-based immunoassays;
- Cell sorting techniques;
- New technologies in microbiology;
- New technologies in molecular biology;

and for the CCL:

- Fuzzy systems;
- Biodynamic modeling in laboratory medicine;
- Communication of laboratory information;
- Integration of laboratory information systems;
- Future of laboratory computing.

The conference language will be English, however, simultaneous translation will be provided for English to Spanish.

There will be a precongress satellite symposium on Wednesday 1 November, at the Hotel Estels, Sitges, on Analytical Quality Assurance in the European Context.

The congress will be held in the Hotel Gran Sitges, Port d'Aiguadolç, 08870 Sitges, Spain. Sitges is situated about 25 kms south from Barcelona. The journey from Barcelona airport to Sitges can be effected by train in about 40 minutes. An airport train runs every 30 minutes from Barcelona Airport Station, but one must transfer at Prat Llobregat Station.

The full registration fee is ESP41 000 before August 15th and ESP46 000 after August 15th. Younger scientists (born before October 1967 – proof will be required at registration) may register for ESP25 000 and ESP30 000, and Accompanying persons may register for ESP10 000 and ESP15 000, on either side of the August deadline. Payment may be made by bank transfer, cheque and credit card. Accommodation can be arranged in the congress venue, Hotel Gran Sitges, and in a number of other hotels, of differing category, near to the congress venue. Details of the hotels are given in the Accommodation Form which accompanies the Registration Form.

A social program will provide an opportunity for participants and their companions to mix, relax and get to know the countryside. A number of social events have been organized, including concerts of classical and folk music, together with a traditional congress dinner.

For further information and registration forms, please contact: Organizing Secretariat, ANT/CCL/SEQC/95, Llançà, 51, 08015 Barcelona, Spain, Tel.: +34 3226 98 27, Fax: +34 3226 69 69

The photograph shows a scene from the Festa Major at Valls, Xiquets de Valls.

International Seminar on Assessment of Carconogenic Risk from Occupational Exposure to Inorganic Substances
17–20 October 1995
European Center (Kirchberg), Luxembourg

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Recently, the assessment of the carcenogenic potential of metals and their compounds has become a contentious issue. However, the ability to assess such risks from inorganic substances is a societal necessity, particularly in the context of workers' health. This topic is also of major importance for industry since the classification of a substance as a carcinogen at international or national levels has serious consequences for both producers and consumers.

This international seminar, structured with plenary sessions, working parties and poster sessions, aims to present as broad a forum as possible for the study of this important health-risk field. There will be three working parties:

- Physico-Chemical Characterization of Exposures;
- Conduct and Interpretation of *in vitro* and *in vivo* Experimental Studies;
- Conduct and Interpretation of Epidemiological Studies.

The seminar will be held at the Jean Monnet Building, European Commission, Directotate-General V, Plateau du Kirchberg, Luxembourg. The seminar will be entirely in English with no translation facilities.

The participation fee will be BEF20 000 for participants from industry and BEF12 000 for other participants. This fee includes: lunches, cocktail, preproceedings, return transfers from hotels to the seminar venue.

For further information, please contact, Mr Emmanuel Chantelot, Seminar Coordinator, EUROMETAUX, 12 Ave de Broqueville, 1150 Brussels, Belgium, Tel.: +32 2775 63 14, Fax: +32 2779 05 23

International Forum on Environmental Catalysis '95 (IFEC'95)
25–27 October 1995
Tokyo, Japan

IUPAC
SPONSORED

This forum has been organized to promote international cooperation and exchange of ideas and information in the research and development of catalytic sciences and technologies which play key roles in global and local environmental issues. With the current global interest in environmental catalysts, and due to the success of the First International Forum on Environmental Catalysis, it was decided to hold a second meeting in this series.

It is hoped that advances in catalytic science will in future improve our environments through, for example, reduction of environmentally unacceptable compounds present in car exhausts. One of the specific topics of this Forum will be a discussion of those catalysts which will directly reduce pollution. The second issue of interest is novel catalytic processes designed to yield valuable products without the formation of polluting by-products – so called environmentally benign catalytic processes.

IFEC'95 will be held at the Chemistry Hall in Tokyo, 25–27 October 1995. The language of the conference will be English.

The conference will consist of three plenary lectures: R. Burch (Reading, UK) *Low NO Options in Catalytic Combustion and Emission Control*; Y. Ono (Tokyo, Japan) *Dimethyl Carbonate for Environmentally Benign Reactions*; and K. I. Zamaraev (Boreskov Institute, Russia) *Catalytic Science and Technology for Environmental Issues*; shorter oral presentations and poster sessions.

To encourage early registration, the advanced registration fee will be JPY30 000 for registrations received before 20 September, thereafter the registration fee will be JPY35 000. Student registration is JPY5000. This registration fee includes the cost of the proceedings which will appear in *Catalysis Today*.

For further information, please contact the Organizing Committee: Prof. Eiichi Kikuchi, General Secretary IFEC'95, Department of Applied Chemistry, School of Science and Engineering, Waseda University, 3–4-1 Okubo Shinjuku-ku, Tokyo 169, Japan, Tel.: +81 33200 5349, Fax: +81 33200 5349, E-mail: ekikuchi@cfi.waseda.ac.jp

Workshop on Soil Chemistry and Ecosystem Health
28 October 1995
St Louis, USA

IUPAC
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Soil is an integral part of the environment. The pedosphere, hydrosphere, atmosphere and biosphere are divisions of the environment which strongly overall and are intimately associated in an ecosystem. Consequently, what happens in the soil should be of considerable interest to all chemists interested in problems of the environment.

SOIL SCIENCE SOCIETY OF AMERICA

The objects of this one day workshop, to be held prior to the beginning of the ASA-CSSA-SSSA meetings, are: (1) to address the impact of soil chemical and biochemical reactions on ecosystem health, and (2) to promote activities of soil chemists, pertaining to ecosystem health, on a global scale. It is hoped that the workshop will serve as a forum for the interaction of soil chemists with other scientists interested in ecosystem health.

For further information, please contact: Dr P.M. Huang, Department of Soil Science, University of Saskatchewan, SK, Canada S7N 5A8, Tel.: +1306 9666838, Fax: +1306 9666881

IX International Symposium on Mycotoxins and Phycotoxins
27–31 May 1996
Rome, Italy

IUPAC
SPONSORED

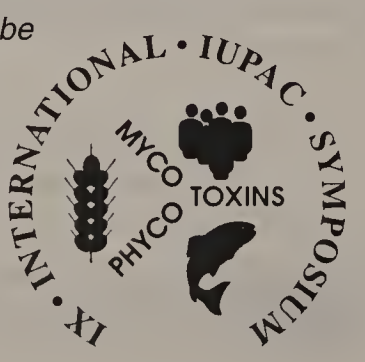
The *Istitutio Superiore di Sanità* cordially invites you to attend the IX International IUPAC Symposium on Mycotoxins and Phycotoxins. The scientific program will consist of plenary lectures, contributed papers (oral presentations and posters) and a workshop. The official languages of the symposium will be English and Italian. The workshop will be conducted in English and French.

There will be three keynote lectures: Global significance of mycotoxins and phycotoxins; Food safety – mycotoxins and phycotoxins in perspective; Overview of international mycotoxin and phycotoxin programs. There will be plenary lectures (parallel sessions) on mycotoxins and on phycotoxins, and contributed papers covering the following subjects:

- Methods of analysis and sampling;
- Toxicity;
- Chemistry;
- Mycology and phycology;
- Biomonitoring;
- Prevention;
- Technology;
- Risk assessment;
- Occurrence.

The FAO/IUPAC Workshop, entitled, 'Practical considerations in food analysis for mycotoxins and phycotoxins', will address the specific needs of developing countries in mycotoxin and phycotoxin analysis.

Further information may be obtained from: Istitutio Superiore di Sanità, Segreteria per le Attività Culturali, Viale Regina Elena, 299, 00161 Rome, Italy



11th International Congress on Catalysis (ICC)
30 June – 5 July 1996
Baltimore, USA

IUPAC
SPONSORED

In 1956, the Catalysis Club of Philadelphia organized the First International Congress on Catalysis, which resulted in the formation of the Council of the International Congress on Catalysis with the objective of perpetuating these meetings. Subsequent meetings have been held around the world, and the 11th such meeting will be held in Baltimore to celebrate the fortieth anniversary.

The 11th ICC will sponsor an equipment exhibit in the Baltimore convention center as an integral part of the Congress. Arrangements for exhibit space rental can be made by contacting E. P. Greenly, American Institute of Physics, 500 Sunnyside Blvd., Woodbury, NY 11797-2999, USA, Tel.: +516 5762441, Fax: +1516 5762481.

All branches of homogeneous and heterogeneous catalysis will be discussed in the conference. The organizers are particularly keen to receive submitted papers that describe novel applications of industrial catalysis, and advances in catalysts preparation and characterization. Papers on the following topics are invited:

- Environmental protection;
- Fuel production and upgrading;
- Production of fine and specialty chemicals;
- Alkane activation;
- Catalyst preparation;
- Catalyst characterization;
- Mechanistic studies;
- Theoretical studies;
- Catalysis by zeolites;
- Polymerization.

The scientific program will consist of five plenary lectures, not more than 135 contributed papers for oral presentation, 30 minutes duration, each presented in three parallel sessions and 300 poster presentations.

All correspondence, except abstracts, should be made to: Dr Kathleen C. Taylor, Physical Chemistry Department, General Motors NAO R&D Center, 30500 Mound Road, Warren, MI 48090-9055 USA, Tel.: +1810 9862010, Fax: +1810 9868697, E-mail: ktaylor@cmsa.gmr.com

Conference Calendar

1995

Applications of the Mössbauer effect

10–16 September
International Conference on the Applications of the Mössbauer Effect (ICAME-95). Rimini, Italy.
Prof. I. Ortalli, ICAME-95, University of Parma, Istituto di Scienze Fisiche, Via M. D'Azeglio 85, I-43100 Parma, Italy. Tel.: +39 (521) 902231. Fax: +39 (521) 236508. E-mail: ICAME95@iprUniversity ofcce.unipr.it

Bioorganic chemistry

17–23 September
3rd International Symposium on Bioorganic Chemistry. Dagomys, Sochi region of Black Sea Coast, Russia.
Dr V. V. Demin, Shemyakin – Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Ul. Miklukho-Maklaya, 16/10, 117871 Moscow V-437, Russia. Tel.: +7 (095) 3351511, 330-6338, 3302800. Fax: +7 (095) 3107007.

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* **14**, 203 (1992).

Chromatography of polymers

18–22 September.
International Symposium on Chromatography of Polymers and Related Substances. Bratislava, Slovakia.
Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, Sk-842 36 Bratislava, Slovakia. Tel.: +42 (7) 3782306. Fax: +42 (7) 375923. E-mail: upoldber@savba.savba.sk or upoldber@savba.sk.

Assessment carcinogenic risk

17–20 October
International Symposium on the Assessment of Respiratory Carcinogenic Risk from Occupational Exposure to Inorganic Substances. Luxembourg.
Dr J. H. Duffus, Director, The Edinburgh Centre for Toxicology, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS, Scotland. Tel.: +44 (131) 4513456. Fax: +44 (131) 4513017.

Environmental catalysis

25–27 October
2nd International Forum on Environmental Catalysis. Tokyo, Japan.
Prof. Eiichi Kikuchi, General Secretary IFEC'95, Department of Applied Chemistry, School of Science and Engineering, Waseda University, 3-4-1, Okubo Shinjuku-ku, Tokyo 169, Japan. Tel.: +81 (3) 32005349. Fax: +81 (3) 32005349. E-mail: ekikuchi@cfi.waseda.ac.jp.

Soil chemistry and ecosystem health

28 October
Workshop on Soil Chemistry and Ecosystem Health. St. Louis, MO, USA.
Prof. P. M. Huang, Department of Soil Science, University of Saskatchewan, Saskatoon, Saskatchewan S7N OWO, Canada. Tel.: +1 (306) 9666823. Fax: +1 (306) 9666881.

Automation and new technology in clinical laboratory

2–4 November
6th International Congress on Automation and New Technology in Clinical Laboratory. Sitges, Barcelona, Spain.
ANT/CCL/SEQC/95, Llançà 51, 08015 Barcelona, Spain. Tel.: +34 (3) 2269827. Fax: +34 (3) 2266969.

Macromolecule–metal complexes

2–5 November
6th International Symposium on Macromolecule–Metal Complexes (MMC-VI). Guangzhou, China
Prof. Chi-Yu Wang (General Secretary), Guangzhou Institute of Chemistry, Chinese Academy of Sciences, Wushan, Guangzhou 510650, China. Tel.: +86 (20) 7708815. Fax: +86 (20) 7705319.

1996

Phenothiazines and related psychotropic compounds

26–29 February
8th International Conference on Phenothiazines and Structurally Related Psychotropic Compounds. Jaipur, India.
Dr R. R. Gupta, 10A Vasundhara Colony, Tonk Road, Jaipur-30218, India. Tel.: +91 (141) 512694. Fax: +91 (141) 515367.

Chemical physics for the 21st century

16–19 April
International Conference on Chemical Physics on the Border of the 21st Century.
Moscow, Russia.
Prof. V. I. Goldanskii, Semenov Institute of Chemical Physics, Russian Academy of Sciences, Kosygin Street 4, Moscow 117977, Russia.

Molecular order in polymers

21–24 May
2nd International Symposium on Molecular Order and Mobility in Polymer Systems.
St. Petersburg, Russia.
Prof. T. M. Birshtein, Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoy pr. 31, St. Petersburg, 199004 Russia.

Free-radical polymerization

26–31 May
2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism.
Santa Margherita Ligure, Genoa, Italy.
Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy. Tel.: +39 (79) 229556. Fax: +39 (79) 229559.

Mycotoxins and phycotoxins

27–31 May.
9th International Symposiums on Mycotoxins and Phycotoxins.
Rome, Italy.
Dr Marina Miraglia, Instituto Superiore Sanità, Food Department, Viale Regina Elena, 299, I-00161 Rome, Italy. Tel.: +39 (6) 4990, ext. 377. Fax +39 (6) 4451767.

Protein folding

17–20 June
International Symposium on Theoretical and Experimental Aspects of Protein Folding. San Luis City, Argentina.
Dr J. Vila, IMASL-Universidad Nacional de San Luis, Ejército de Los Andes 950, 5700 San Luis, Argentina.

Surface forces

25–29 June
11th International Conference on Surface Forces. Moscow, Russia.
Dr L. B. Boinovich, Institute of Physical Chemistry, Leninsky Prospect 31, 117915, Moscow, Russia.

Organic synthesis

30 June – 4 July.
11th International Conference on Organic Synthesis.
Amsterdam, Netherlands.
Conference Secretariat ICOS – 11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (80) 234471. Fax: +31 (80) 601159.

Catalysis

30 June – 5 July.
11th International Congress on Catalysis. Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520–8286, USA. Tel.: +1 (203) 432 4378. Fax: +1 (203) 432 4387.

Chemical education

14–19 July
14th International Conference on Chemical Education – Chemistry: Expanding The Boundaries.
Brisbane, Australia.
Dr W. Beasley, Graduate School of Education, The University of Queensland, Brisbane, Queensland 4072, Australia.

Sweeteners

14–20 July
International Symposium on Sweeteners. Jerusalem, Israel.
International Symposium on Sweeteners, PO Box 50006, Tel.:- Aviv 61500, Israel. Tel.: +972 (3) 5140014. Fax: +972 (3) 5175674 or 5140077. E-mail: 100274.2665@CompuServe.COM.

(Bio)degradable polymers

15–18 July
37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects.
Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy.

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.
Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

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Front cover: Guildford: location of the IUPAC General Assembly, August 1995.

International Union of Pure and Applied Chemistry

New Techniques in Materials Science: Force Microscopy

It would probably be an under-estimation to say that the force microscope is revolutionizing the study of materials and interfaces. Whereas previously one made measurements on laboratory-sized samples and inferred something about what could be happening at a microscopic level. One can now directly probe interfaces and manipulate individual atoms on clean surfaces (see Figs 1–3).

The principle of a force microscope is straightforward, one moves a microscopically sharp tip of a hard material, for example, silicon nitride, over a very clean surface keeping the tip as close as possible to that surface. This tip is attached to a finely balanced cantilever arm. This cantilever arm is electronically balanced in a heterodyne feedback loop so that any minute displacements are measurable. Consequently, as the arm moves over the surface the various surface irregularities are 'mapped out'. Various experiments in air, liquids and in ultra-high vacuum have demonstrated atomic resolution and exceptional stability even under general laboratory conditions (Figs 1–3). The first scanning microscopes were built in the early 1980s and earned Ernst Ruska, Gerd Binnig (both German) and Heinrich Rohrer (Switzerland) the 1986 Nobel prize in physics. However, they quickly left the rarefied world of the physics laboratory for the harsher reality of the chemistry laboratory.

At a fundamental level, the subtle interactions between the tip and the surface are also being investigated. For example, the hard tip rests on the surface, but what is the actual distance from the tip to the surface atoms? This will be determined by the balance of attractive and repulsive forces operating at the interface. Typically, in such experiments, one is examining

Fig. 1 Image of the Si(111) 7 × 7 structure showing an area of the surface of 10 × 15 nm. Atomic resolution is clear.

Fig. 2 Atomic steps on a cleaved GaAs (111) surface.

the modulation of the interaction forces which operate at 2–30 nm from the surface atomic layer. One is able therefore to probe irregularities of the surface layer of molecules or atoms, that is, how the surface layers are arranged, which may well be different from the bulk arrangement as determined by X-ray or neutron diffraction techniques. Or, one may investigate how the balance of the attractive and repulsive forces between the tip, which may be chemically modified, and the surface, which may also be chemically characterized, vary as a function of chemical composition and modification. Figure 4 shows a surface force apparatus, this is a modified force microscope where both surfaces are smooth, and one is interested in measuring the dynamics normal and parallel to the interface between the two surfaces as a well-characterized mechanical modulation is applied.

A variant on a force microscope is a scanning tunneling microscope (STM). In an STM, a current flows through the substrate from the tip, which is charged, and one monitors the current flow as the tip scans irregularities on the surface – the other electrode. There is thus a great similarity, perhaps one should rather say, complementarity between a force microscope and a tunneling microscope. Both probe interfaces and interfacial phenomena, however, one responds directly to modulation in surface–tip interactions and the other to surface-tip conductivity.

Some of the most recent experiments with a scanning tunneling microscope have shown its potential for imaging molecules on clean metal surfaces. For example, the irregularities of a clean gold surface can be mapped out with a force microscope, steps and terraces being readily observed. If the tip maintains a constant separation from the outermost gold atoms then

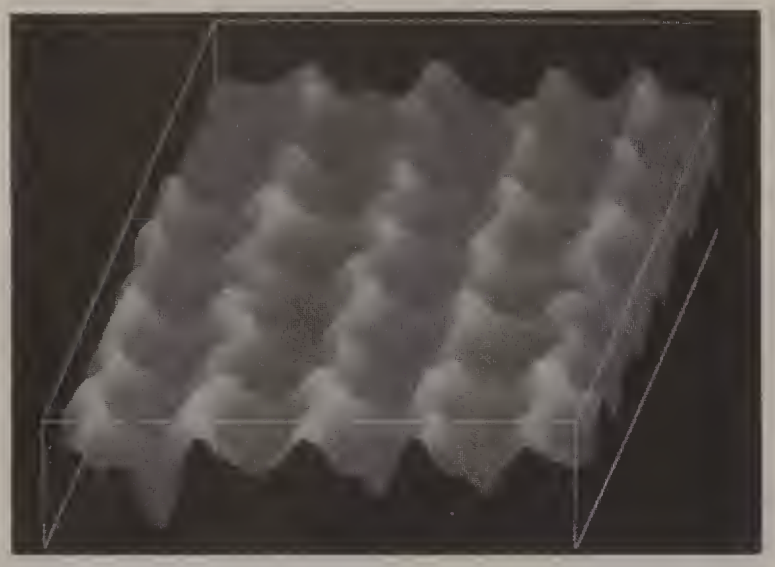


Fig. 3 Constant current image of a graphite surface (2.5 × 2.5 nm) in air.

the current flowing will be modulated by the atoms on the flat surface, however, if a benzene molecule or even a strand of DNA are lying on this surface then their dielectric properties will modulate the current flow and they will be detected and their shape observed.

The ability to investigate the surface of a metal, and also to investigate molecules adsorbed onto a metal surface, has been cleverly demonstrated by Manfred T. Reetz and colleagues at the Max-Planck-Institut für Kohlenforschung, Mülheim, and Forschungszentrum Jülich, Jülich, Germany (*Science* **267**, 367 (1995)). Scanning tunneling microscopy (STM) and high-resolution transmission electron microscopy (TEM) have been used to determine the dimensions of a series of palladium clusters stabilized by tetra-alkylammonium salts. Electrochemically prepared colloids were used in which the average diameter of the inner metal core was varied between 2 and 4 nanometers and the size of the ammonium ions were adjusted in the series $^{+}N(n\text{-}C_4H_9)_4 < {}^{+}N(n\text{-}C_8H_{17})_4 < {}^{+}N(n\text{-}C_{18}H_{37})_4$. The difference between the mean diameters of the metal cluster, with its associated alkane sheath, as determined by STM and by TEM allows the determination of the thickness of the adsorbed protective layer.

Although there is much current interest in metal clusters because of their actual and possible catalytic properties, there is a problem in stabilizing such reactive entities in solution. Various polymers have been used, but the question remains, how do the polymer molecules attach themselves to the naked metal core and how thick are these protective sheaths? High-resolution TEM can be used to measure the diameter of the metal core, the high-energy electrons are strongly scattered by the electron-rich metal atoms and one may determine the mean diameter of the cluster's core. However, molecule adsorbed onto the surface of the cluster contain a much lower electron density and consequently scatter the incident high-energy electrons less well than the metal atoms. Thus, TEM is not a useful probe of the surface layer of these clusters. However, the STM probes, in detail, the surface of a nanoscale object. Although the polymer molecules at the surface are stable and unreactive, they will exert a strong influence on their immediate vicinity. Thus, a measure of the attractive forces operating between the arm of a tunneling microscope and a polymer coated metal cluster can readily be made and interpreted in terms of the total diameter of the coated cluster. Then, the difference between the cluster diameter as measured by TEM (d_{TEM}) and that measured by STM (d_{STM}) gives directly the thickness of the polymer coat.

In this way Reetz *et al.* have determined the sheath thickness for a variety of different sheath molecules and of different preparative conditions. Indeed, on the basis of these studies they have proposed a model of the geometric properties of ammonium alkane salt-stabilized palladium clusters. They also make suggestions as to the mechanism of electron-tunneling seen in these materials.

In a scanning tunneling microscope, the tip is charged and only a few nanometers from the surface and will therefore exert an enormous electric field on the molecules of the surface and in the bulk near the surface. Due to the mechanical stability required to make a force microscope work, the tip may be translated, relative to the surface, with extreme precision. Thus the distorting influence of the tip may be used to distort the surface in such a way as to engineer or create lines of changed substrate. For example, a large crystal of a liquid crystal (large polarizable molecules), can be distorted by moving the charged tip of an STM over the surface (the surface may be scratched) in such a way as to produce channels millimeters in length, but only tens of nanometers in cross-section, of material where the organization of the molecules is different from that of the bulk. The intense electric field generated by the proximity of the charged tip (a potential of 10 Volts between the tip of the probe and the substrate will give an electric field of 10^{10} V/m for a 1nm probe-tip separation) having caused the molecules, nearest the moving tip, to re-order their three dimensional arrangements (the interaction energy, E_{int}, between an applied electric field, E, and a molecule of polarizability, α, is, $E_{int} \approx \alpha E^2$ giving for $\alpha = 40 \times 10^{-40}$ Cm^2 an energy of interaction of 241 kJ mole^{-1} – more than enough energy for localized structural changes) thereby giving channels within the solid where the local dielectric constant, and hence the local refractive index, are different from that of the bulk, i.e. well-defined and reproducible waveguides.

It is well known that at large distances molecules attract one another; the mere fact that solids and liquids exist is a manifestation of this fact. Likewise, the observed finite densities of solids and liquids tells us that at some critical intermolecular distance, molecules begin to repel one another. The balance point between

these attractive and repulsive forces defines the architecture of solids and the mean molecular separation in liquids. There is however, a difference between adhesion at a molecular level and adhesion in engineering. There is no doubt that molecules of solids stick together and can be separated mechanically. The problem is explaining the connection between molecular interactions and mechanical measurements at interfaces. A rational theory of these phenomena should be based on the theoretical concept of reversible work of adhesion and on the measured quantity of adhesion energy, which includes the energy necessary to restructure the interface as the surface moves.

It is from studies of adhesion that the force microscope has greatly developed. It was observed that two smooth surfaces would spontaneously jump into contact when brought sufficiently close together. For example, two ultra-smooth pieces of mica, gold, polymer or solid gelatin solution cannot be held apart when their separation becomes small enough, typically a few nanometers. The tip of a force microscope can be thought of as a surface – it will not be atomically sharp, and will have a rounded end. The tip will therefore be attracted to the surface and this attractive force will be modulated by any material between them. Likewise, if the molecular surfaces of the tip and the surface proper are modified then the measured interaction force may also be modified. This technique has been widely used in recent years for probing adhesion, lubrication and frictional forces across a surface, as well as mapping functional group microstructure in polymers and binding/recognition interactions in biological systems.

In surface-force studies one can investigate directly both the static and dynamic forces between smooth macroscopic surfaces, see Fig. 4. As with AFMs, forces are determined from the observed deflection of a spring, and displacements are measured using some optical interferometric, electrical or strain-gauge tech-

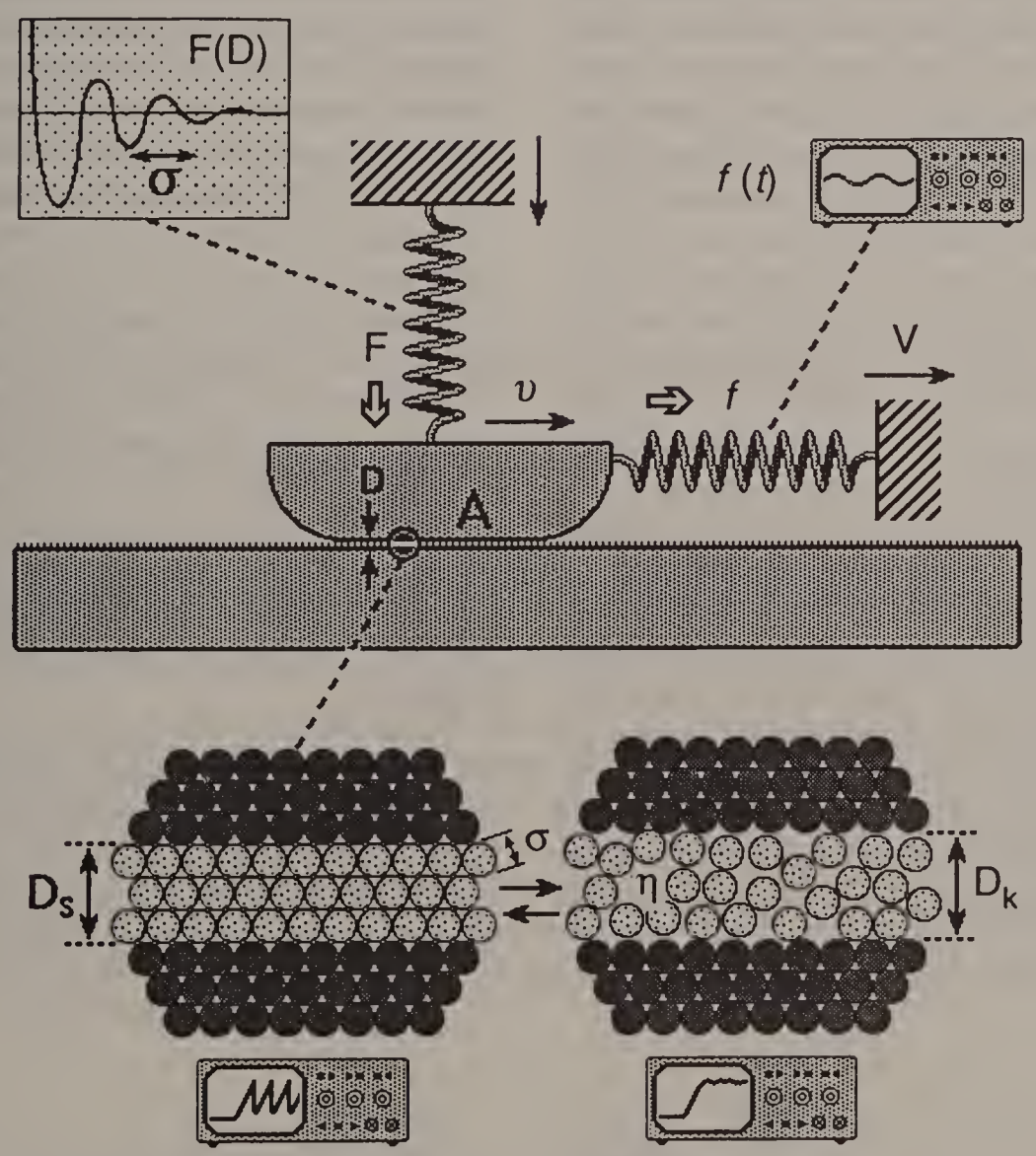


Fig. 4 Principle of a surface force apparatus for measuring the normal force, *F*, and the shear or friction force, *f*, between two clean smooth surfaces, area *A*, separated by a fluid film of thickness *D*. An optical interferometer allows the separation of the surfaces to be monitored with high precision. Typical contact areas are 100 μm^2, and gap thickness can range from one molecular layer ($D = \sigma = 0.4$ nm, where σ is the mean molecular diameter) to hundreds of nanometers. An oscillatory force-function, *F*(*D*), is typically measured across simple liquids is shown at top-left, and two common types of friction traces (friction force vs. time – *f*(*t*)) are shown on the oscilloscope traces. During sliding, two smooth surfaces usually remain in one of the adhesive minima of the force function, although the kinetic thickness, D_k, is usually slightly different from the equilibrium or static thickness, D_s, with η being the shear-induced fluid viscosity. (Image courtesy of *Nature*, 374 607–616 (1995)).

nique. The intermolecular interaction potential, or force function, between two surfaces interacting in or across a liquid medium can be attractive, repulsive or even oscillatory. Recent studies have revealed that the structure of the liquid molecules, and of the confining surfaces, are important in determining what will be the nature of the force function. Furthermore, two crystalline surfaces may induce a confined liquid to solidify, freeze, when the gap thickness is close to a small multiple of the molecular diameter, see Fig. 4 bottom-left.

The force between two surfaces across a liquid or lubricant fluid tells us whether two surfaces, when pressed together, will come into adhesive contact or remain separated by a thin fluid-like layer. Such experiments have a profound impact on our understanding of tribology and, indeed, of engineering. For example, only one layer of water molecules, 0.25 nm thick, between two hydrophilic surfaces can be sufficient to reduce the interfacial friction to very low values. If the surface–fluid interactions induce crystallization of the lubricant, then the measured friction will be of the stick-slip type. That is, it will not be a smooth function of the interfacial separation, sticking of the two surfaces will occur when the lubricant freezes, when additional force is applied slipping of the surfaces will occur in the shear-induced molten state. Such effects are now believed to underlie many other apparently unrelated dynamic processes involving stick-slip motion, such as earthquakes, the sound of a violin, and even sensory perception – taste and touch (B. Bhushan, J. N. Israelachvili and U. Landman, *Nature* **374**, 607–616 (1995)).

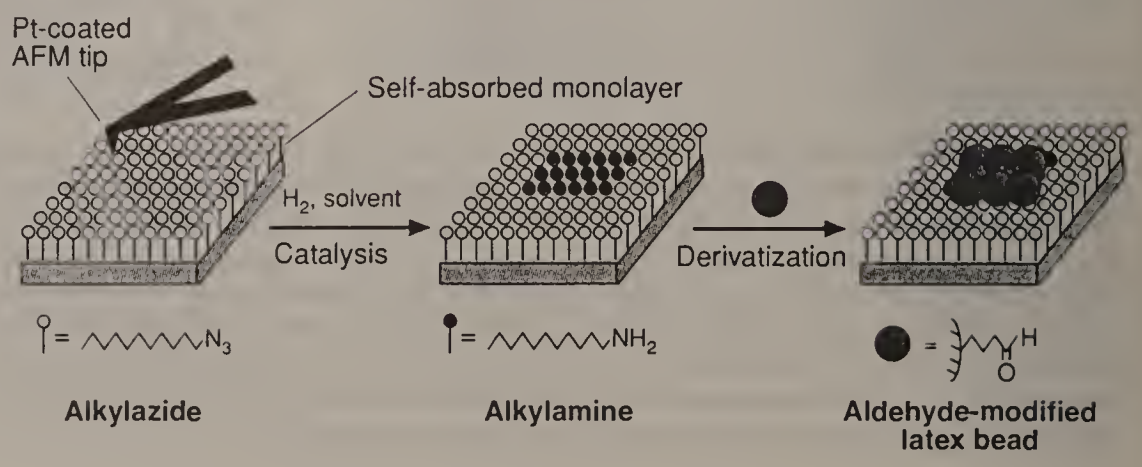
Previously, however, it was nearly impossible to correlate changes in friction with specific chemical interactions between the surface of the probing tip and the other surface. This difficulty results from the chemistry of the force microscope's tip changing during a scan, atoms and molecules at one surface may well exchange with those on the other surface. Thereby altering the way the surfaces interact. This suggests, however, that the measured magnitude of the frictional force on the tip is directly proportional to the magnitude of the interaction potential between the tip and the surface.

The group of Charles M. Lieber, Harvard, USA, have recently tested this hypothesis, that is, if specific functional groups were attached to the two surfaces would it be possible to rationalize the measured interaction. The team produced tips that were covalently modified with self-assembled monolayers which terminated in either hydrophobic methyl ($R\text{-}CH_3$) groups or hydrophilic carboxylic acid groups (R-COOH). These tips were then used to measure the forces at surfaces coated with the same methyl or carboxyl terminating monolayers.

When a clean uncoated tip is used to probe the friction at a surface of methyl and carboxyl terminating groups, no difference between the two very different types of surface is seen. The $-CH_3$ and -COOH groups are structurally similar, similar size and similar polarizability, and the probing bare tip cannot discriminate between the two chemically distinct surface molecules. However, when a carboxyl terminating tip is used to study a surface of carboxyl and methyl groups, the carboxylic acid terminating regions of the surface exhibited greater, by a factor 3, friction than the methyl group terminating regions of the surface. When a methyl terminated tip is used, the friction contrast is reversed.

The observed trend in adhesive forces between the variously terminated tips and surfaces is consistent with expectations that the interaction between polar hydrophilic groups, capable of forming hydrogen bonds, will be stronger than that between non-polar hydrophobic groups. When a modified tip is scanned across a surface patterned with $-CH_3$ and -COOH groups in a defined arrangement, interactions between the tip and the surface are revealed as differences in the measured frictional force. These modulations in friction are translated into differences in contrast on micrograph images that reveal regions with different chemistry.

Lieber points out that the principle is quite general. It should be possible to map the spatial distribution of other types of functionality such as charged or chemically reactive groups with this approach. Chemical force microscopy might also be of use in the study of specific interactions such as those between comple-



Nanocatalysis occurs on self-absorbed monolayer. Scanning with platinum-coated atomic force microscope (AFM) tip catalyses hydrogenation of terminal azides to amino groups, which are amenable to further derivatization (adapted from *C&E News*).

mentary and non-complementary oligonucleotides or between ligand-receptor pairs (*Science* **265**, 2071 (1994)).

This explosion of interest and research on small-scale structures and individual atoms and molecules has extended to every branch of chemistry, including biochemistry, and materials science. Indeed, it has lead to a renaming, a reclassification, of chemistry; previously used terms now seem to be prefixed by 'nano' thereby creating whole new scientific fields. One such is nano-catalysis. This new branch of catalysis research has been created by a group of chemists at the University of California, Berkeley. This group have succeeded in carrying out highly localized chemical catalysis on a coated surface, thereby creating new high-resolution structures on the surface.

The Berkeley team, lead by Peter G. Schultz, combined atomic force microscopy with molecular self-assembly in their study of nano-catalysis. However, this group coated the AFM tip with platinum. This platinum coated tip was the precision catalysis device. Previously, force microscopes had been used to manipulate individual atoms on a surface – to construct words, messages or company logos. However, with a high-precision tool for inducing catalysis in a particular part of a large molecule or between two molecules one has made a significant advance over bulk heterogeneous catalysis. To demonstrate the new technique (*C&EN April 17, 1995*), see Fig. 5, Schultz and his coworkers an alkylazide self-assembled monolayer on a glass surface. They fabricated the catalysis probe by evaporating a 7 nm layer of platinum onto a silicon AFM tip that had been coated with an adhesion layer of chromium.

Scanning the Pt-coated tip over the surface of the terminal azide groups results in catalytic hydrogenation of the azides to amino groups. These amino groups can then be selectively modified with a variety of reagents to generate different structures. By labeling the generated amino groups, the Berkeley group was able to show that 10% of the surface azides were catalytically converted into amino groups.

Force microscopy is a rapidly expanding field of research. Hardly an issue of *Nature* or *Science* appears without a new application for such devices in areas as diverse as probing molecular arrangements at surfaces, or reading and writing molecular information at surfaces. The ease of access to such equipment and their reliability, they are now commercially available 'black boxes', make these microscopes invaluable for the study of new solids.

Biophysical Environmental Chemistry:
A New Frontier for Chemistry

Jacques Buffle

This paper discusses the position and role of environmental chemistry. It discusses the various aspects of environmental chemistry and emphasizes the need for developing fundamental studies in biophysical environmental chemistry in order to better understand the functioning of environmental systems. These systems include a large number of structures, from nanometer to meter, which play key roles on compound fluxes, and consequently on the homeostasis of ecosystems and on their disturbance by anthropogenic activities. Both structures and fluxes are presently ill-defined and new concepts and methods must be developed. For chemistry, this is a challenging area where supramolecular structures and processes play dominant roles. It is also a challenging field for the development of environmental sciences since detailed knowledge of physicochemical processes are needed in macroscopic modelling of compound circulation in ecosystems. In addition, teaching this discipline would allow students to better confront complex, structured real systems.

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Introduction

Not all scientific disciplines have reached the same level of maturity. Today, environmental chemistry parallels the emergence of biochemistry in the first half of the present century. The evolution of a scientific discipline involves several steps: formulation of concepts, collection, classification, and interpretation of data, and generalization and formulation of new more rigorous

and quantitative concepts. Both chemistry and biochemistry have passed through long descriptive periods in which important discoveries allowed one to deduce structures, and properties of elements and compounds. This led to quantitative formulation of modern concepts allowing predictions to be made on compound reactivity. Whereas the descriptive phase in chemistry has probably reached its pinnacle, in biochemistry a great deal still has to be done. This lag is due to the greater complexity of the system studied and, importantly, to the key role played by supramolecular organized structures.

Environmental chemistry deals with more complicated systems than biochemistry, and it is a younger discipline; despite the development of sophisticated modern analytical techniques, it is still at its infancy. That is, much work has still do be done on experimental data collection and classification. Consider sediments, soil aggregates or humic compounds which are key environmental components, but whose rigorous chemical description is complex. However, such complexity does not mean that rigorous description of environmental systems is impossible – biochemistry has succeeded in describing in detail the primary to quaternary structures of proteins, polysaccharides or DNA, and of even more complicated structures such as biological membranes, even though such achievements were considered as impossible at the beginning of the century. Thus environmental chemistry will eventually succeed in describing the components and structures that play key roles in environmental processes. However, to achieve such a synthesis much time will be required, and new sophisticated technologies and concepts should be developed. In particular, it is crucial to realize that environmental chemistry is more than just an application of 'classical' chemistry concepts and methods. Most of the latter have been developed for chemical systems composed of small molecules, often with only a few components. Similarly, most analytical techniques have been developed for homogeneous systems, so that, physically complicated systems should initially be transformed (by preliminary steps such as filtration, dissolution of solid phases or extraction) into well homogenized systems for a meaningful interpretation of data. Although such a classical chemical approach has been, and is still useful in environmental sciences, it is not sufficient to understand the chemical basis of environmental system functioning which largely depends on physicochemical processes based on the existence of biological and physical *structures* and of corresponding *concentration gradients* and *fluxes* of compounds. This is again exemplified by means of the analogy with biological systems: the chemical analysis of an homogenized biological cell gives some information on its composition, but little on its functioning.

The goal of this paper is to emphasize this particular aspect of environmental chemistry which may be less familiar to the reader and which is called, hereafter, biophysical environmental chemistry to suggest the important role of supramolecular physicochemical structures and their links with biological activity. We believe that this aspect of environmental chemistry should be developed to allow, ultimately, efficient environmental protection. To clearly point out the peculiar features of this aspect of environmental chemistry, we compare it with classical environmental chemistry based on the application of well-established general chemistry and chemical analysis concepts to environmental systems. The term classical chemistry is used here to distinguish it from biophysical chemistry. This comparison should help distinguish the role of environmental chemistry from amongst the other environmental sciences and other chemical disciplines.

The place of environmental chemistry in environmental sciences

A simplified but useful representation discriminates between three aspects of all environmental natural sciences (Fig. 1): the understanding of the functioning of unperturbed environmental systems (boxes 1 and 2), and the understanding of anthropogenic perturbations on these systems (box 3). It is essential to make the distinction between aspects 1 and 2, on the one hand, and 3 on the other: anthropogenic perturbations cannot be understood and controlled without a preliminary understanding of the behaviour of unperturbed ecosystems. A major role of environmental chemistry therefore is to study the physicochemical processes occurring in unperturbed environmental systems.

It is also useful to discriminate between environmental microprocesses, occurring at small scales – nm to mm (box 1), and macroprocesses, large scales – mm to km (box 2) corresponding to whole ecosystems. Fig. 1 shows that in both cases their investigation should be undertaken in association with microbiology and geochemistry. Although the border between these two scale ranges is arbitrary, the nature of the corresponding processes, the techniques used to study them and, consequently, the corresponding conceptual approaches are very different.

Traditionally, environmental chemistry has developed in nonchemistry departments. Consequently, the development of environmental chemistry has been largely driven by nonchemical disciplines interested in macroscopic aspects of environmental sciences (box 2), and hence classical chemistry concepts valid for well-mixed systems, as well as classical analysis applicable to homogenized samples, have been and are still, by far, the most widely used. In particular, such approaches are those applied to quality monitoring in

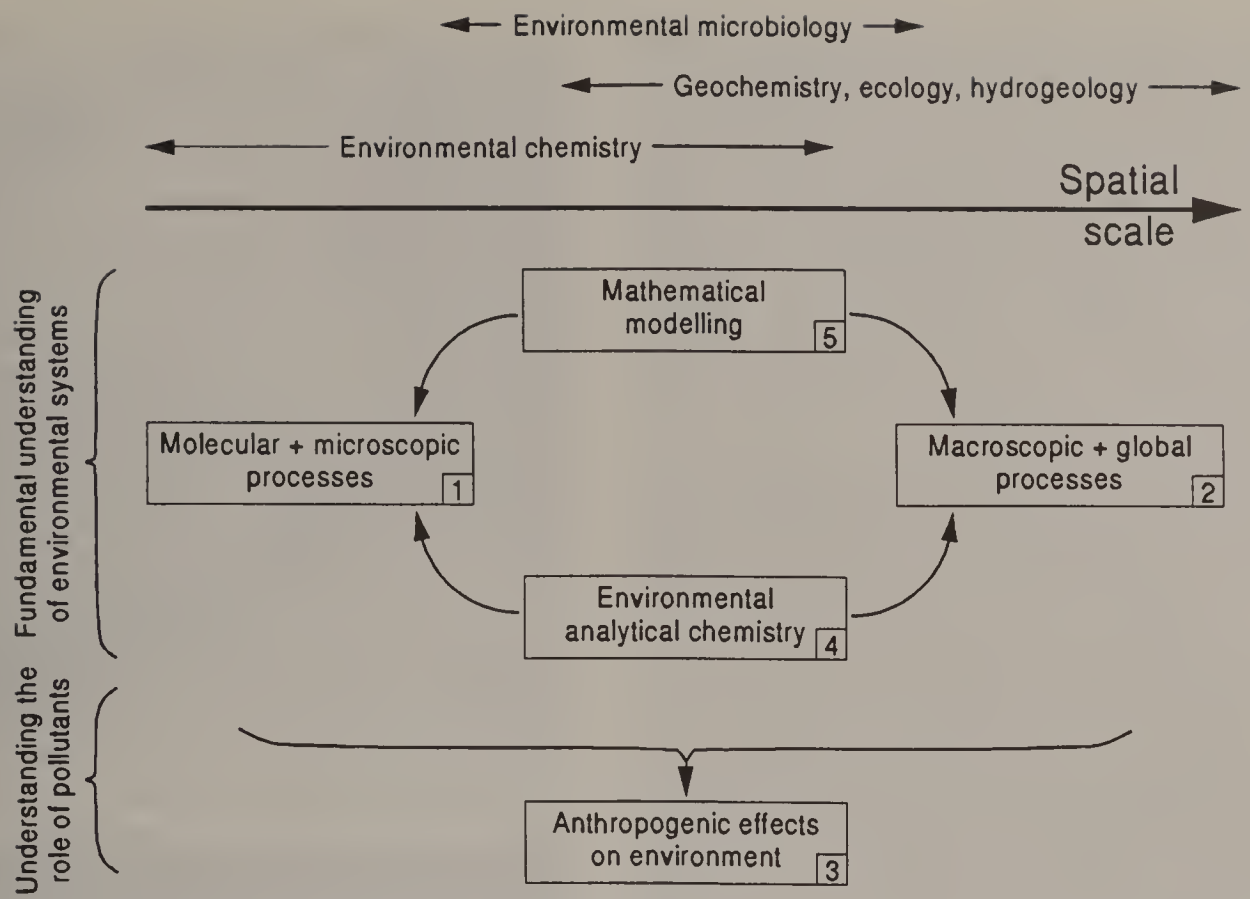

Fig. 1 Different aspects covered by environmental natural sciences

governmental institutions. Such approaches have their uses, but environmental chemistry should not be restricted to this classical approach, as it is not sufficient to provide the necessary concepts and information for developing predictive models of ecosystem functioning. Complementary studies on molecular and microscopic structures and related processes (box 1), i.e. biophysical environmental chemistry, are also required. Such studies require long-term physicochemical investigations, with sophisticated techniques and high-level biophysical, biochemical or physicochemical competence which are generally only available in chemistry and biochemistry departments. Therefore, full development of environmental chemistry should include the biophysicochemical approach as well as the aforementioned classical aspects.

Another task of environmental chemistry is to develop the analytical chemical methods (box 4) needed to study environmental processes (boxes 1 and 2) and allow environmental quality monitoring (box 3). Since chemistry influences many geological and biological processes, these methods are not only required by chemists but also by most other environmental scientists. Analytical chemistry has thus a key role to play in almost all aspects of Fig. 1.

Due to the urgency of solving pollution problems, most organizations favour the founding of strategic short-term, empirical, studies. Because of the key role that environmental chemists have to play in developing analytical methods for environmental quality monitoring, they are under a strong pressure to move progressively from fundamental studies on biophysicochemical processes to tackle short-term problems related to environmental management. There is here a real danger for the future. Urgent pollution problems must be solved, but one should not forget that for the long-term basic research is the most useful – and it pays off.[1] By favouring short-term empirical studies on the environment, the authorities discourage thorough-minded scientists to undertake fundamental studies in this field, thus hampering environmental science to develop into a sound science. This may have dramatic consequences for the future generations, which will be confronted by more serious pollution problems than our own, but who will have no rigorous scientific discipline to solve them.

Specificity of biophysical environmental chemistry as a chemical discipline

Study of environmental biophysicochemical processes

As far as physicochemical processes are concerned, work conducted over the last 20–30 years has shown that global geochemical cycles of elements are ultimately controlled by the reactivity and physicochemical properties of compounds at the molecular level, and that, without a good knowledge of the behaviour of chemical compounds at this level, no prediction is possible at a global level. The cycling of phosphorous in lakes is an interesting example of an old problem, which is, as yet, without a satisfactory quantitative model.[2] This is because phosphorous cycling depends on many largely ill-defined physicochemical mecha-

nisms such as transfer of phosphate through biological membranes, oxidation of organophosphorous compounds, phosphate adsorption on iron hydroxide, nucleation of iron phosphate, oxidation of iron(II) into iron(III), calcium phosphate crystal formation, growth and dissolution which itself may depend on adsorption of surface active organic compounds, etc. Each of these steps is intricately related to other physicochemical processes, in a manner analogous to the metabolic cycles in biochemistry.

The primary role of biophysical environmental chemistry is to elucidate the most important mechanisms, at the molecular and microscopic level, in particular, those which play a rate limiting role in the overall cycle of the element of interest. The aforementioned microprocesses are examples of systems rarely studied in detail in macroscopic nonchemical disciplines and which would be more easily tackled in chemistry or biochemistry departments. Only then will it be possible to model the corresponding physicochemical processes to include them as submodels in global models of ecosystem functioning. Presently, most global models include physical, biological or geochemical macroprocesses, but they rarely include detailed microprocesses, because of the dearth of available data. As a result, global models often fail to represent adequately detailed spatial distributions or seasonal evolution of many chemical compounds. Conversely, in cases where such detailed studies of physicochemical, and/or microbial studies have been made, good concordance between experimental and predictive calculations are obtained, for example, the fate of herbicides in the Rhine River after Schweizerhalle accident.[3]

In contrast to traditional systems studied in chemistry, environmental chemistry systems have the striking feature that many of their properties are closely related to their physical and chemical heterogeneity. The study of environmental physicochemical processes therefore requires adopting new conceptual approaches which combine classical chemistry concepts with, for example, reactivity probability concepts and supramolecular structural physical models. The main features characteristic of biophysical environmental chemistry are.

1 The *chemical heterogeneity* of environmental systems is a difficulty for nonenvironmental chemists who are usually trained to think in terms of reactivity of individual, small molecules. According to this approach, the study of a complex mixture consists in first detailing each component of the mixture. The complexity of environmental systems, however, is huge and complete characterization is never possible. Even if one casts aside the enormous efforts required to study environmental problems in this manner, solutions to the questions posed are not always obtained. Indeed, this approach ignores that heterogeneity itself is a key property of the environmental systems of interest. Fulvic and humic compounds of soil and waters provide a good example of such a case. Even after purification, fulvic and humic samples are composed of a large number of similar, but not identical compounds. As an ensemble, they act cooperatively as a complexing system for metal ions (and small organic molecules), with significant buffering intensities spanning an extremely wide concentration range of metal ion. As such, they play a key role in maintaining acceptable concentrations of vital and toxic metal ions for organisms in soils and waters.[4–6] Alone, none of the individual molecules will impart this property. Hence they should be thought of as a single chemical system rather than as a mixture of individual compounds. It has been shown that the overall properties of heterogeneous chemical systems may be rigorously related to the properties of individual molecules by introducing the concept of reaction probability.[6–8] Descriptions of such chemical systems should then be based on rigorous statistical concepts, applicable not only to a large number of identical molecules, as is usually done in classical thermodynamics, but also to a system consisting of a large number of similar but nevertheless not identical molecules. Similar approaches are applicable to some of the chemical properties of whole soils and sediments.

2 It is now well established that the most important reactions in environmental systems (soil, sediment, ocean, fog droplets) occur at solid-liquid and gas–liquid *interfaces*. The electric field and solvent structure are very different at these interfaces (over a thickness of tens of nm) than in the bulk solution and thus may drastically modify the nature and rates of chemical reactions.

3 Interfaces are the simplest examples of *environmental microstructures*. All environmental systems, at all levels, are physically structured – from nm to km. Examples of large structures are: soil horizons; and lake, ocean or atmosphere stratification. Microstructures are those which environmental chemistry is more concerned with. Aggregates between large polysaccharide macromolecules, clays and micro-organisms in soils, water, and sediments (or dust particles in the low troposphere) are examples of microstructures in the range nm to mm (Fig. 2). They play a key role, for example, in the circulation of oxygen and water in soils, indeed, of most nutrients in the biosphere, and therefore exert key influences on the maintenance of life. Sediment–water interfaces in lakes and oceans are another example. They are stratified at the μm to mm level (Fig. 3) in successive layers of varying chemical composition, which controls the overall exchanges of chemicals between the bulk water and the sediment. Similarly, the gas exchanges between the ocean and the atmosphere (such as that of CO_2 with its link to climate change) are predominantly controlled by a diffusion layer of 30–80 μm thickness whose chemical composition is very different

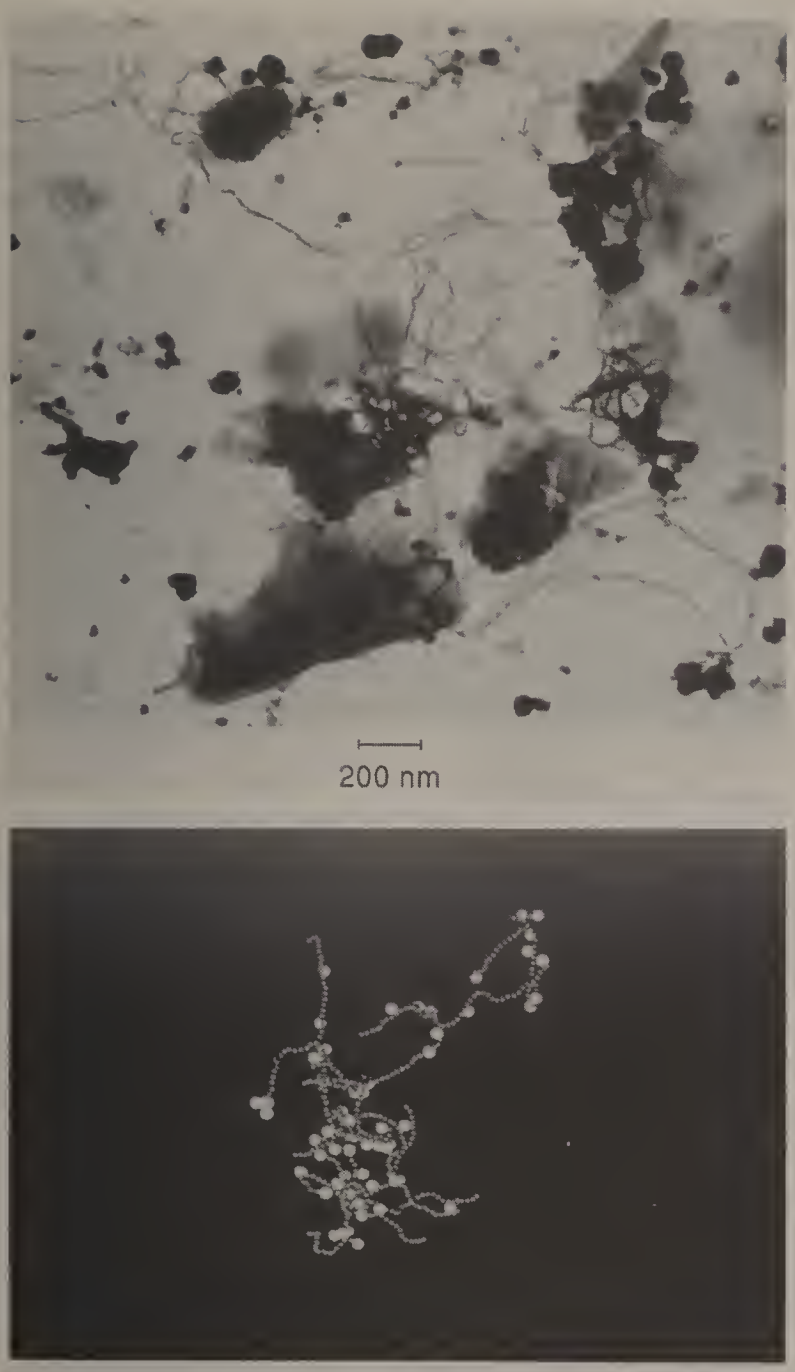

Fig. 2 (a) Iron hydroxo-phosphate globules (spherical black particles with size < 0.2 μm) formed at the oxic-anoxic boundary layer of a eutrophic lake. These globules are aggregated with other colloidal material, filaments, and bacteria (not visible in this figure), which influence the sedimentation rate and bioavailability of iron and phosphate. (b) Kinetics of aggregation between spherical colloids and comparatively larger filaments or macromolecules can be simulated by numerical modelling. The iron globules of (a) have well-defined chemical composition, and transmission electron microscopy shows that they are themselves aggregates of small units (1–2 nm in size), possibly the precursor shown here

from the bulk solution. In all cases, the functioning of living environmental macro- and microsystems is dependent on their physicochemical structure; indeed the functioning of living systems (organisms or ecosystems) is based on pH, redox and other chemical gradients which can only develop with physical heterogeneity. A good characterization of environmental microstructures is therefore a key task of environmental chemists (as characterization of cell structure is a key aspect in biochemistry).

4 The physical structures existing at all scales of environmental systems and the corresponding chemical gradients imply the existence of *fluxes of compounds* within the system of interest, e.g. soil aggregate, or between one compartment and the neighbouring compartment, sediment–water interface. Environmental systems are therefore dynamic systems. Thus understanding environmental processes necessitates coupling kinetics of chemical reactions with physical transport processes. This often occurs by molecular diffusion in microsystems, e.g. soil or underground pore water, as well as by eddy (turbulent) diffusion and laminar or turbulent hydrodynamic flow, at the macroscopic level (e.g. lakes, rivers, atmosphere).

It is essential to realize that properties related to items 1–4 above, in combination with classical chemical reactions, are key factors for the maintenance of the *homeostasis* of environmental systems. They also correspond to processes of environmental systems which are particularly sensitive to impacts of anthropogenic activities. These concepts should then be taught in detail to future environmental scientists, and even given at a general level to chemistry students, so that they could take them into account during their professional life.

Environmental analytical chemistry

Analytical chemistry, i.e. development of new analytical methods based on new physicochemical principles, is a well-established branch of chemistry. However, environmental sciences requires the development of new analytical methods specifically adapted to the physicochemical nature and properties of the environmental systems of interest. Much work has been done to solve problems for environmental applications, by combining careful sampling and sample handling to sometimes very sophisticated instrumental techniques, such as ICP-MS, GC-MS, HPLC-MS, Flow Field Flow Fractionation techniques, NMR and FTIR, or Surface analysis techniques (e.g. Particle Induced X-ray Emission, Laser Microprobe Mass Spectrometry, X-ray Fluorescence or Electron Energy Loss Spectroscopy, etc.). In most cases, however, the sample structure is destroyed and an average analysis obtained. Such analyses cannot give any information on the links between chemical composition or properties and sample structure.

As discussed above, what is specific to the environment is that ecosystems are dynamically and physically nonhomogeneous. Monitoring the concentration of compounds is not sufficient for quality control; concentration gradients which occur over distances sometimes smaller than millimeters are also key parameters for making predictions on chemical fluxes within or between environmental compartments. This implies developing new specific methods enabling to perform *in situ*, remote sensing of these fluxes, without perturbing

environmental systems either by chemical contamination or by physical disturbance.[4] This will also allow continuous monitoring of chemical parameters, in real time, which is required for efficient pollution control. The development of such systems has recently become feasible. For instance, devices have been built which allow one to determine oxygen, anions or trace metal concentration profiles at the sediment–water interface, while keeping a resolution of 100 μm, i.e. that corresponding to the strata thicknesses on the top sediment layer (Fig. 3).[9] Another example is the development of NO_x sensors with very fast response time for recording NO_x concentrations in the low troposphere. Such fluctuations are directly linked to eddy diffusion processes, and provide more precise estimates of NO_x fluxes than gradients based on classical concentration profile measurements.

Fig. 3 Fine chemical stratification at the top sediment of sediment–water interface in an anoxic lake. The two layers correspond, from top to bottom, to manganese oxide, and iron oxide formed in situ on Teflon plates inserted vertically in the sediment. Picture is obtained by electron microscopy coupled to mapping by energy dispersion spectroscopy. Layers are a few millimeters thick and the separation zone between the two layers (marked with the vertical bar) is 100 μm reflecting very steep vertical redox gradients in the sediment. Transmission electron microscopy shows that the iron oxide layer is composed of either amorphous iron hydroxide globules (similar to those of Fig. 2a) or crystallized lepidocrocite, depending on lake pH (neutral or acid, respectively). The exact nature of these layers influences phosphate and many other trace compound fluxes between water and sediments

Another specific aspect of environmental analytical chemistry is related to speciation. Bioavailability, and consequently, toxicity of any particular element or compound for a micro-organism depends both on its flux inside the microecosystem surrounding the organism and on its chemical form, so-called chemical species, e.g. redox state, complexation with natural ligands, etc.[10] Presently, most of the upper concentration limits of toxic compounds are fixed by rather arbitrary governmental regulations, imposing a maximum tolerable average total concentration of the compound in the ecosystem of interest. Chemical speciation in particular is often not considered because of the lack of data or adequate analytical technique. Development of non-perturbing speciation analytical methods coupled to detailed biophysicochemical environmental studies are therefore a prerequisite for building sound ecotoxicological regulations.

Teaching and research in environmental chemistry

The position of environmental chemistry in a faculty of sciences

From the above, both for research and teaching, there is a need for two types of environmental chemistry (without a clear-cut boundary between them):

- The first type has been called here classical environmental chemistry, including classical environmental analytical chemistry. It may be incorporated in nonchemistry departments and its role is not to form front-line chemical research, but to apply modern well-established methods and concepts for solving macroscopic environmental problems, by knitting closely with other scientific disciplines.
- The second type corresponds to biophysical environmental chemistry and advanced environmental analytical chemistry as discussed above. It should be dealt with in biochemistry or chemistry departments, by specialists in biophysical, physicochemical or biochemical processes, trained to apply these concepts and methods, and develop new concepts for environmental systems.

Classical environmental chemistry can be taught at various levels to chemistry or nonchemistry students interested in general environmental sciences, with a view to working on multidisciplinary studies of the effect of anthropogenic impact. Biophysical environmental chemistry should be specifically taught to chemistry and biochemistry students. We believe that such teaching is of vital importance for environmental chemistry (and environmental protection), and is also a key training for chemistry students since they have little opportunity to confront complicated structured systems in the remainder of their curricula.

Role of modelling

In recent years, the use of numerical simulation models, as a means to evaluate large-scale or complex natural processes, has increased sharply. In some cases, the predictions generated by these models are considered as a basis for public policy decisions (e.g. global circulation models to predict Earth climate). There is, however, an overemphasis on the predictive value of modelling. Even by neglecting the fact that all models are oversimplified compared to natural processes, many natural processes are still unknown and, above all, the primary value of models is heuristic. The prediction capability of models then should never be the main goal of modelling. On the other hand, it is unquestionable that models have enormous importance as educational tools both for students and researchers. They allow: (i) classification of information, (*ii*) checking working hypothesis with experimental data, (iii) formulation of new hypothesis by eliminating unimportant factors, and (iv) sensitivity analysis.

These considerations apply to all disciplines. But, as a means of learning, modelling is particularly important in environmental chemistry: it is the only tool available to rapidly evaluate the indirect, but sometimes predominant influence, on the macroscopic evolution of ecosystems, of factors which affect molecular or microscopic processes. Let us take again lake eutrophication as an example: it depends on a number of molecular or microscopic processes such as formation rate of iron hydroxide species like that shown in Fig. 2, its reactivity with phosphate ions, its aggregation processes to form microscopic globules and more complicated aggregates, and their sedimentation. Although each step must be studied experimentally, only mathematical simulation, combining microscopic and macroscopic processes, allows understanding the respective role of each of them on the overall evolution of the lake. In general, the time and space domains of chemical processes are very far away from those occurring at the macroscopic or global scale in environmental systems. It is thus extremely difficult, both for students and researchers, to assess the actual importance of chemical processes on ecosystem evolution – modelling is thus an extremely useful tool. It is also helpful for nonchemists to learn the importance of using detailed physicochemical processes instead of empirical parameters to make reliable quantitative predictions.

Experimental work

Expertise in any scientific discipline can only be acquired by working experimentally in that field. This is even more important in environmental sciences because of the complexity of environmental systems and the multidisciplinarity of the problems involved. As far as environmental chemistry is concerned, the student should be confronted, at least, with the following three experimental aspects:

- Study of physicochemical processes *in situ*. Planning and performing well-controlled experiments in the field is much more difficult than in the laboratory, because of the large number of factors to be considered and controlled in order to allow sound interpretation of data.
- Study of biophysicochemical processes in the laboratory with model compounds simulating natural systems. Studies on natural systems allow one to discriminate between predominant and secondary factors affecting a particular macroscopic process. However, results of *in situ* measurements cannot provide precise values of physicochemical parameters. These can only be determined in the laboratory, by using model experimental systems to mimic natural systems.
- Development in the laboratory, and application *in situ,* of analytical methods specifically designed for studying environmental processes. Measuring the right parameters under correct conditions is a key issue in order to understand natural processes. This is far from being trivial in complicated and structured natural systems, and often significantly more complicated than with well controlled systems, in laboratory conditions.

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Syllabus for a Short Postgraduate Course in Medicinal Chemistry

C. Robin Ganellin

A compilation of subject headings for 24 lectures is provided as the basis of a short course for teaching the elements of medicinal chemistry. This course is aimed at organic chemists who have recently entered the pharmaceutical industry and wish to become conversant with medicinal chemistry. Such courses have been successfully running as 1-week summer schools in the UK, USA, and Netherlands.

In developed countries, the pharmaceutical industry is one of the major employers of organic chemists especially in research and development. Many prospective chemist employees are hired to become medicinal chemists or to fit into a team of scientists engaged in the search for a new drug which it is hoped will become a new medicine.

The newly appointed chemists have to discover how to synthesise new molecules for biological testing. This may make full demands on their synthetic skills, but it may not be fully satisfying intellectually. It will certainly not provide research medicinal chemists with a fully rewarding intellectual experience if they cannot appreciate fully the reasons for making these compounds. Consequently, they will have to learn to communicate with biological scientists, to converse with biochemists, pharmacologists, toxicologists and pharmacists in order to be actively involved in drug design. They will want to decide which compounds to make, as well as appreciating how to make them.

Soon the novice medicinal chemist will come up against the mystery of trying to relate chemical structure to biological activity. In this connection, colleagues will mention the importance of lipophilicity, hydrophobic interactions, quantitative structure-activity relationships (QSAR), molecular modelling, electrostatic energy potentials and so on. These may be unfamiliar words and new concepts that will be difficult to acquire and take time to comprehend. Few organic chemists will have taken courses in drug design during their university training. Some may have taken courses in natural product chemistry or bioorganic chemistry but these topics will be of little help in tackling structure-activity analysis. What then can be done to assist the new employee enter this new field of endeavour?

There is debate among medicinal chemists about the best way of teaching the subject. The Medicinal Chemistry Section Committee[1] of IUPAC has set up a Working Party to consider a Medicinal Chemistry Curriculum. The Committee sent a questionnaire, regarding academic training for medicinal chemists, to major research pharmaceutical companies in a variety of countries. One set of replies, mainly from Germany, Japan and the UK, have been analyzed and the results published.[2] Responses from Italy and the USA which were solicited subsequently were similar to those received earlier. The overwhelming response (>90%) was that companies seek to hire the best organic chemists and whether they have, or have not, received some education in medicinal chemistry was of secondary importance. This confirms the impression that there is a strong need to introduce the novice medicinal chemist to further education in medicinal chemistry. The Committee has responded by proposing the subject matter for a one-week school.

Some pharmaceutical companies are aware of these problems and run their own courses in drug design; often they encompass some introductory pharmacology and biochemistry which relates directly to their own research areas of interest. It was in recognition that there may exist such a need that the Royal Society of Chemistry (RSC) introduced, as an experiment, in 1979 – a one week Summer School[3] in medicinal chemistry as part of their general program of one week courses in specialist topics.

One cannot, of course, teach a whole subdiscipline in one week. However, if the topics are carefully chosen to represent the core of the subject, and if it is well lectured by active practitioners, it should be possible to get across most of the main concepts and increase the awareness and understanding of the specialist language. Such a short course can provide a basic framework, the sense of direction of which the chemist can then build upon if prepared to put in the necessary reading and study. With the above thoughts in mind, the second Summer School in medicinal chemistry was organized by Dr A. M. Roe and Dr C. R. Ganellin in1981.

What then should constitute the syllabus for such a one-week school? The approach taken was to focus on the core discipline of medicinal chemistry, namely structure-activity analysis and to take in related con-

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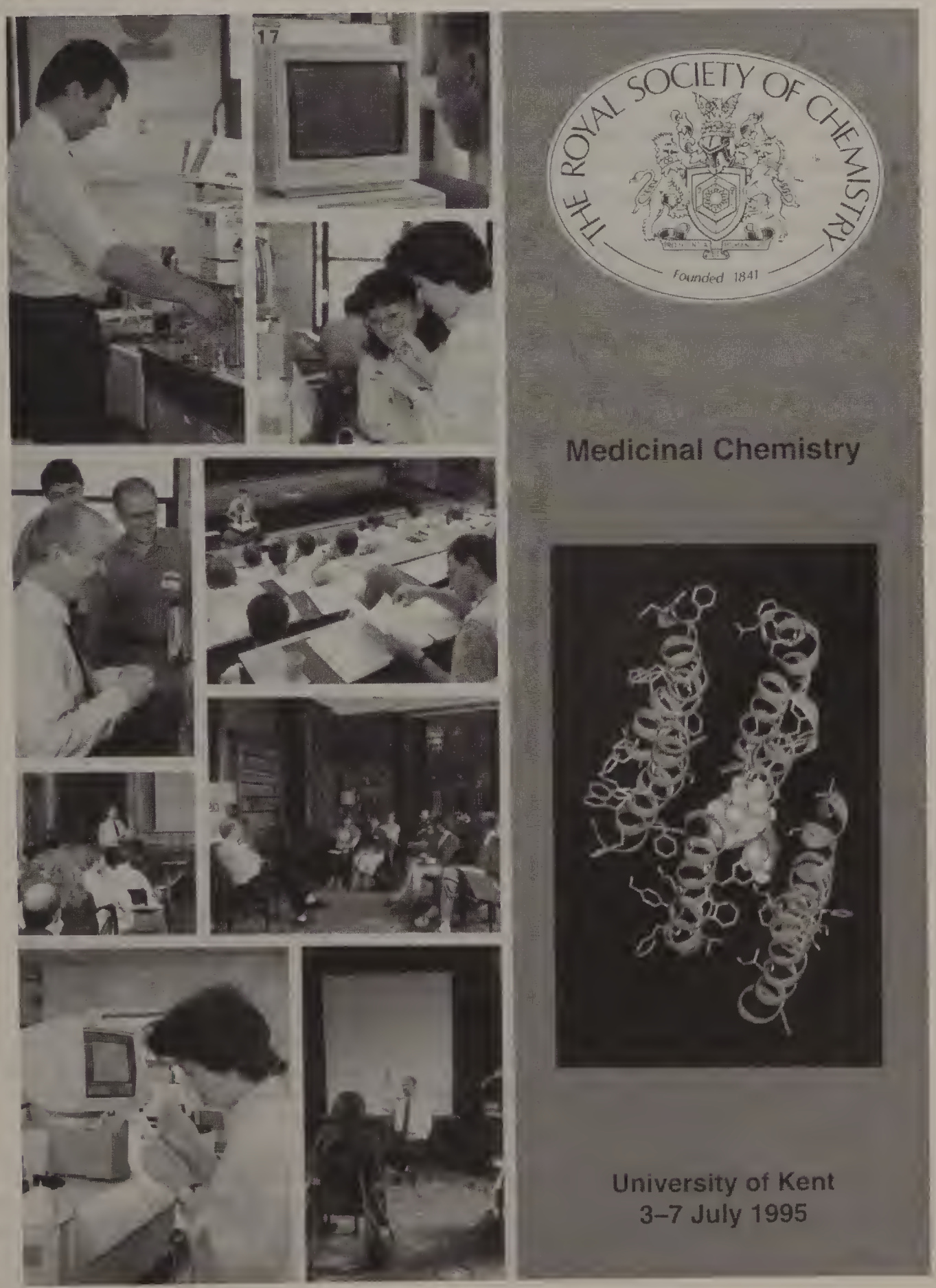
cepts and provide a few examples. Because of time constraints, there was little background history included and almost no discussion of diseases as targets for research. The course was also directed to graduate or postdoctoral organic chemists who had recently entered the pharmaceutical industry or were contemplating doing so in the near future.

The course was successful and established the blueprint for a syllabus which has subsequently been running, in alternate years, at the University of Kent, Canterbury, under the auspices of the RSC.[4] Always fully subscribed (100 places for 'students') with about 20 lecturers (mostly from industry) it has clearly demonstrated its utility. To emphasize this point, it is noteworthy that similar 'schools' have subsequently been established in other countries. In the USA (at Drew University, Madison, NJ, annually since 1987, 100 places) in the Netherlands (at Leiden, Amsterdam in Noord-



Details of the RSC School of Medicinal Chemistry held last year

wijkerhout since 1992, 20 places) and most recently in Switzerland (Leysin, since 1994, 20 places). The exact content of these different schools varies according to the lecturers and the perception of the organizers, but basically they have a very similar composition.

The author has been approached many times about the best course content for a medicinal chemistry school, especially by medicinal chemists from other countries who wish to see something of a similar nature established in their own country. It seems of interest and appropriate therefore, to share the thoughts of the IUPAC Medicinal Chemistry Section Committee with a wider audience and to solicit comment from interested chemists.

A week's course is encapsulated in the following list of subject headings representing approximately 24 lectures. By and large, they also reflect the most popular topics suggested by the company responses to the questionnaire,[2] namely subjects such as biochemistry, drug metabolism, pharmacokinetics, pharmacology and physiology, computer modelling and QSAR. However, additional components for drug design are included such as the importance of physiological concepts, operational strategies, prodrugs and case studies of drug discovery. Naturally, these subjects can all easily be expanded to fill several weeks if desired.

Syllabus for a 1-week school as an introduction to medicinal chemistry

Introduction

- Research Strategy.

Biological targets

- Lead generation/sources for drugs;
- Receptors and drug–receptor interactions;
- Enzymes and design of inhibitors;
- Ion channels, membranes and transporters;
- Second messengers.

Bioassay

- Screening methods and the information that they provide;
- Determining activity: principles of pharmacological assay, biological variation (and the need for statistics), *in vitro* and *in vivo* methods.

Structure-activity methods

- Physicochemical concepts, including pKa, solvent partition, Hammett, H-bonding, steric parameters;
- QSAR, parameterization and computer assisted lead optimization, statistical methods;
- Molecular modelling, energy calculations and molecular graphics;
- Operational strategies in molecular modification, pharmacophore identification, conformational restriction, isosterism, lipophilicity control, solubilization;
- Development of a lead compound (a tutorial exercise).

Biodisposition and implications

- Pharmacokinetics, concepts, parameters and modelling;
- Drug metabolism;
- Prodrugs;
- Molecular toxicology and avoidance of toxic intermediates.

Case studies

Three case studies of drug discovery and design.

Four lectures selected from the following possibilities:

- Bioorganic chemistry;
- Chirality in drug action;
- Clinical pharmacology;
- Combinatorial chemistry;
- Drug delivery;
- Ethical considerations;
- Molecular biology; role in drug discovery;
- Nucleotides;
- Patents;
- Peptidemimetics;
- Regulatory procedures.

References and notes

1. Membership of the Committee comprises Professor J. G. Topliss (President), Dr N. Koga (Vice-President), Professor W. D. Busse (Secretary), Professor C. G. Wermuth (past-President), Professor C. R. Ganellin (Chairman of the Working Party), Professor L. A. Mitscher. Additionally involved were Dr P. Lindberg (Astra, Hässle, Mölndal, Sweden), Professor G. Tarzia (University of Urbino, Italy), Dr J. Ide (Sankyo, Tokyo, Japan) and Professor A. Monge (University of Navarro, Spain)
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3. Held at University of Bradford and organized by Professors J. M. Midgley and J. B. Stenlake.
4. Enquiries should be directed to Ms L. A. Hart, The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN.

New names and addresses pull-out

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The President's Report

K. I. Zamaraev

Lessons of 75 years of activity and perspectives for the future

This biennium is of special importance for our Union. In 1994 the world community of chemists celebrated the 75th anniversary of IUPAC. This gave the Union a opportunity to look back over its history and to see more clearly both its strong and weak points. By giving due appraisal to its achievements, and appropriate criticism to its failures, we may better understand how the Union should operate in the future.

K. I. Zamaraev

Achievements in IUPAC activities

During the 75 years of its history, our Union has faced many dramatic events, but it has always been able to overcome them successfully and with dignity.

The objective of IUPAC is to contribute to the advancement of pure and applied chemistry in all its aspects. Among various accomplishments of our Union, particularly appreciated by the world community of chemists, are its contributions to the creation of self-consistent nomenclature, terminology, quantities, and units in various fields of chemistry. When taken together, these recommendations comprise what may be called the international language of chemistry.

Another major achievement of IUPAC is in the area of codification, which is closely related to nomenclature, and standardization. All over the world, chemists use IUPAC reference books and tables in various fields of chemistry, for example, the reference book on electrochemical potentials or tables of rate constants for reactions in the atmosphere. I have noticed that quite often chemists from both academia and industry use such reference books and tables without realizing that they have been prepared and reviewed by IUPAC panels composed of internationally respected experts.

A further major achievement of our Union, in the past 75 years, has been its remarkable ability to provide, through its publications and the network of IUPAC-sponsored conferences, the chemists of the world with the possibility to work as a team even under extreme political conditions. The Union survived World War II. In 1940 it was still acting, in 1944 it resumed its activity. In the period of the 'Iron Curtain', IUPAC continued to serve as a unique channel for international cooperation in pure and applied chemistry. Whatever the political situation, chemists from every country, be it USA or USSR, Egypt or Israel, Ethiopia or Republic of South Africa, were equally and warmly welcomed at IUPAC-sponsored conferences all over the world.

Still another major achievement of the Union during its 75-year history, is the creation, through the membership of its Divisions, Commissions, Committees and other bodies, of a world-wide network of independent experts in nearly all fields of chemistry.

Let me express my sincere admiration of these people who have worked and continue to work hard in the Union as volunteers, for the benefit of the world community of chemists. As we all know, they are, for all intents and purpose, not paid for their work, since both the income and expenditure of the Union are minimal. It is of interest to note that the largest, compared to other countries, annual subscription paid to the Union, that of the USA, which is the country with the biggest annual turnover of its chemical industry, would be sufficient to support only two postdoctoral positions in that country.

The results obtained by the Divisions/Section and other IUPAC bodies after the General Assembly in Lisbon (1993) are summarized in the written reports of the Divisions/Section Presidents and Chairmen of the relevant bodies, which the delegates of the Council have in their files. From these reports one can see that during the last biennium the scientific business went on within the Union more or less as usual, apart from a few important exceptions which will be discussed below.

Criticism of IUPAC activity

Today, we live in a rapidly and dramatically changing world. It is therefore perhaps not surprising that, in spite of impressive achievements in the past, as outlined above, during recent years IUPAC has become subject to increasing amounts of criticism for certain limitations in its organization and activity. These criticisms have come from both within and from outside of the Union.

Whereas many scientific bodies within IUPAC still remain satisfied with their own activity and the present structure of the Union, the IUPAC Council, Executive Committee, and many of the Bureau members have expressed criticism of the Union's organization and activities. Selective external refereeing of some IUPAC projects and of its activity in general, suggests that this criticism is, perhaps, shared by the chemistry community at large, including chemical industry.

For example, such criticism has been expressed in the 1993 Vice-President's Critical Assessment of IUPAC Activity by Prof. H. A. Staab.

Briefly, the main points of his criticism, and that of others, are:

1 The content of many IUPAC projects, their planning, fulfilment and evaluation suffer from such drawbacks, for example, low priority with respect to real challenges currently facing the international chemistry community. Criticisms on related points include:

- lack of international significance of certain projects undertaken by IUPAC, indeed, what is it about a project which necessitates the involvement of IUPAC;
- lack of careful enough advanced planning;
- too long a time required for completion of a project;
- lack of adequate procedure for evaluation of project quality at all stages from initiation to completion.

2 The present structure of the Union is too rigid to provide the flexibility needed to respond to the rapidly changing modern world of chemistry.

3 The quality of the biennial IUPAC Congresses often does not match the high standards expected from the Union. Relatively few IUPAC-sponsored conferences cover the 'hottest' frontier areas of modern chemistry.

4 Official publications of the Union are not always of the quality that is expected from IUPAC. The impact factor of *Pure and Applied Chemistry* has today became lower than that of many other multidisciplinary international journals, which cover various areas of chemistry, such as *Accounts of Chemical Research* or *Angewandte Chemie*. *Chemistry International* is often criticized for being too much an IUPAC in-house magazine with insufficient articles interesting for the chemical community at large.

5 Insufficient visibility of IUPAC in the eyes of the world chemical community outside the Union, including industry.

Response to criticism and restructuring of the union

The above-mentioned criticisms have been taken seriously by some IUPAC Divisions, its Bureau, Executive Committee and the Officers of the Union. Certain measures have been implemented to improve the performance of the Union. They are presented below, numbered in the same way as the corresponding drawbacks listed above:

1 In April 1995, the Executive Committee decided to ask all the Divisions/Section once again to look critically at their current and proposed new projects. They were advised that, starting with the General Assembly in Guildford, only those projects of international significance, that is, a significance which necessitates the involvement of IUPAC, should in future be initiated. The following projects addressing problems of international significance are being initiated in 1995 through the Pool of Titular Members (see below): (i) Oil spill clean up (ii) Remediation of heavy element contaminated sites (iii) Alternative scenarios for future energy production.

In 1995, the Task Force on Scientific Aspects of the Destruction of Chemical Warfare Agents of the Organic Chemistry Division published a report on its activity, including the recommendations of international importance.

2 During the last 8 years, important efforts have been made towards restructuring the Union. Among the measures taken during the present biennium the following should be noted:

- creation of a Pool of Titular Members, which is specially designated to carry out, within a limited period of time (usually 2 years), projects suggested from both inside and outside the Union which are deemed to be of highest priority;
- bringing more flexibility into the distribution of Titular Members ('zero sum') between various Commissions and projects within the Divisions/Section;
- proposals for the reorganization of the *Applied Chemistry Division* into a *Division of Chemistry and the Environment*, and of the *Clinical Chemistry Division* and *Medicinal Chemistry Section* into a *Division of Chemistry and Human Health*. These proposals, which initially came from the President of the Applied Chemistry Division, have been discussed within the Union, and are expected to come forward for approval by Council at Guildford.

Under the agenda item 'Changes to Statutes and Bylaws', the delegates of the Council can find in their files additional proposals by the Bureau (Executive Committee) aimed at simplifying the membership hierarchy within the Union, and to bringing more democracy into IUPAC by giving the Associate Members full voting rights. These measures will help to speed up the rotation of membership within Commissions, when there is a need to rapidly start projects in new important areas. The Executive Committee has also suggested that, during their meetings in Guildford, the Divisions/Section should devote a substantial amount of time to discussing their future activity and to making recommendations on possible further restructuring of the Union. When speaking to the Council at Guildford, the Divisions/Section Presidents were requested to speak

mainly on these two issues. The Executive Committee itself held at Guildford a special 'brain-storming' meeting on these issues.

3 At the request of the Bureau, Profs. J. Jortner and G. Modena, recently prepared proposals on how to improve the scientific quality of the biennial IUPAC Congresses. The organizers of the 1997 Congress have been requested to start following these recommendations. From 1999, the IUPAC Congresses are planned to be organized back-to-back with the IUPAC General Assemblies, as suggested two years ago by Prof. Staab. The Executive Committee expects this action to provide better overlap between the scientific and business activities of IUPAC.

The Divisions/Section Presidents and Bureau still have to give more thought on how to improve the list of IUPAC-sponsored Symposia by introducing more frontier areas. In my view, it is important that Noble Prize laureates should be specially invited to participate more actively in the Congresses and other IUPAC-sponsored conferences, as well as in actual IUPAC projects. A good example here was the participation of Profs. J.M. Lehn and G. Porter in the 'Science for Life' Forum, organized jointly in Brussels in 1994 by IUPAC and the European Chemical Industry Council to mark the 75th anniversary of IUPAC.

4 During the General Assembly at Guildford, I plan to discuss with the Publication Committee the possibility to organize refereeing of the texts of plenary and invited lectures from the IUPAC-sponsored conferences that are published in *Pure and Applied Chemistry*, as is normally done by non-IUPAC journals when they publish similar material.

5 Special efforts have been made during the last few years by some IUPAC bodies and its Officers to improve the visibility of the Union, for example,

- organization by Vice-President Prof. A. E. Fischli and the Committee on Chemistry and Industry of a series of regional Forums and national events under the headings 'Science for Life' and 'Chemistry for Life' to commemorate the 75th anniversary of IUPAC;
- rapidly evolving cooperation with UNESCO in several projects to help developing countries; this cooperation was started by Vice-President Fischli and Secretary General den Boef, and three IUPAC Divisions are already contributing to this effort;
- continuation of the CHEMRAWN programme with the CHEMRAWN IX Conference on *The Sustainable Production, Use and Disposal (including Recycling) of Materials* to take place in 1996 at Seoul;
- continuation of the monograph series on 'Chemistry for the 21st Century', through volumes on Stereocontrolled Organic Synthesis, Chemistry of the Atmosphere, and Ultrafast Processes in Chemistry and Photobiology published between the General Assemblies in Lisbon (1993) and Guildford.

Perspectives for the future

What do the above statements about the achievements and drawbacks of IUPAC imply for the future of the Union?

First, the so-called 'core' activity (chemical nomenclature, codification, and standardization) should remain as one of the milestones of IUPAC activity on the international scene. Major new areas of chemistry are rapidly emerging, and will, I believe, continue to appear with no less rapidity in the 21st century. Among such rapidly evolving areas is, for example, the so-called supramolecular chemistry – a field that covers a gap between the 'usual' chemical compounds and complicated biological structures. Another example is a vast area of chemical substances and materials, such as fullerenes and their derivatives, small metal and oxide particles and layers with special structure and properties, that are in between the 'usual' chemical compounds and the composite structures of today's materials science. I believe that relevant IUPAC bodies should immediately organize teams of experts who could work professionally on nomenclature and symbols in these areas. In this work, IUPAC must establish closer relations with such world-recognized international and national bodies, dealing with nomenclature and standardization in chemistry, such as CODATA, the Chemical Abstracts Service of the American Chemical Society, and US National Institute of Standards and Technology, Beilstein (Germany), and VINITI (Russia).

An important task is to finish the work on the nomenclature of the already discovered transfermium elements. This should be done in close cooperation with the relevant National Adhering Organizations and in strict compliance with the IUPAC Statutes and Bylaws.

I feel that the chemistry community at large, including chemical industry, often takes IUPAC activities in the field of internationally agreed nomenclature and standardization for granted. This is why it sometimes seems to underestimate the importance of IUPAC for this particular activity. One can imagine, how much money it would cost the national chemical societies and industrial companies if various national communities could not agree on a joint nomenclature and would, for example, use different symbols to denote the same element. A lot of money would be spent in this case to translate the chemical knowledge obtained in one country, into the language of chemistry used in another one – much more than these countries pay today as their subscriptions to IUPAC.

In my opinion, the second milestone of IUPAC activity in the future must be the analysis of the chemical aspects of globally important issues, such as environmental problems, future production of energy and materials in the context of sustainable development and human health. Here, the role of the Union may be that of

an international organization, standing firmly on a scientific foundation independent from governments and industry, with a world-wide network of experts in various fields of chemistry. Due to this structure, IUPAC can make independent judgements on important issues that are touchy or sensitive for the general public, governments, and industry. IUPAC should not act here as a judge, but should critically evaluate the various factors for and against a particular issue. It should indicate both potential dangers and possible uncertainties in estimating these dangers.

Another important task of the Union is to participate in improving the image of chemistry in the eyes of the general public by demonstrating through, for example, the CHEMRAWN programme, and the monographs on 'Chemistry for the 21st Century', how great may be the benefits that mankind can obtain from a properly used knowledge of chemistry and from its application in chemical industry.

It is important to note that in the future such projects could. perhaps, be partly financed by UNESCO, UNIDO, private funds, as well as by governments and industry. However, if financed by the latter two sources, the Union must make it quite clear that IUPAC would not accept to be placed under any pressure from the donors, and will guarantee a fair treatment of a problem.

One more important task for the Union to accomplish, is to establish closer cooperation with various international organizations that tackle the problems of global importance. A good example here is the already-mentioned cooperation of IUPAC with UNESCO in projects aimed to help developing countries. I think that the Union should make greater efforts to elect its representatives to the top positions in various international organizations working on global issues. In this context, we are pleased to note the recent election of Prof. V. A. Koptyug – the IUPAC representative to the ICSU Scientific Committee on Problems of the Environment (SCOPE) – as Vice-President of that important body. I hope this will help the Union to become more actively involved in SCOPE projects involving chemistry.

Conclusions

Overall, the achievements of IUPAC notably outscore its shortcomings. Moreover, in my opinion, many IUPAC members already see how to overcome these shortcomings. This makes me optimistic about the future of our Union. However, hard work is needed from all IUPAC members to make this optimism a reality.

Finally, I would like to express my most sincere thanks to all the members of IUPAC who have worked with dedication in the Union during the past 75 years, and in particular during the present biennium. I have enjoyed working with Vice-President Albert Fischli, Past-President Allen Bard, Secretary General Gerrit den Boef, and Treasurer John Ward. My special gratitude is to the Executive Secretary, Dr Mo Williams, former Deputy Executive Secretary Ann Troughton, and the members of the Secretariat staff for their hard work for the Union. For Dr Williams this is the last General Assembly in which he participates as the Executive Secretary before retirement in April 1997. During his service as the IUPAC Executive Secretary for more than a quarter of a century, Mo Williams has made an enormous contribution to the work of the Union. Therefore, he deserves today our special thanks.

Secretary General's Column

Gerrit den Boef

This will be my last Secretary General's column, and it will deal with the progress made at the General Assembly in Guildford in August 1995.

It is true to say that significant progress was made at Guildford towards the goal of the scientific renewal of the Union. For many years, we have been talking about restructuring our scientific activities, and although progress has been made, the pace at which this occurred has not satisfied everybody, in particular, those who are concerned about the lack of awareness of the Union in tackling important problems in which chemistry is involved and to which the Union, because of its unique position, can contribute in achieving solutions. In April 1995, the Executive Committee, stimulated by a critical review by the US Academy of Science, once more discussed the then current situation and concluded that at the General Assembly in Guildford a special effort should be made to increase the momentum in this process of scientific renewal of the Union. A letter to that effect was sent to all scientific bodies of the Union in May again emphasising that a number of projects undertaken within IUPAC suffer from a number of weaknesses. For example:

- have a low priority;
- are not suitable activities for IUPAC, but are pieces of research or reviews, which although of scientific interest, should and could be better undertaken by a research group in a chemical laboratory;
- have taken too long for completion.

Indeed, looking critically at the reports of our projects

Gerrit den Boef

published in *Pure and Applied Chemistry*, quite a few of them suffer, in the opinion of amongst others the Executive Committee, from one or all of these weaknesses.

During the restructuring efforts of the past 8 years, attempts have been made to improve the situation by trying to involve external refereeing of ideas for new projects, thereby obtaining the opinion of the whole chemical community. However, in practice this has only marginally resulted in a better visibility of the Union.

One could, of course, ask whether the visibility of the Union should be our first priority. The answer to that question is that the chemical community at large, indeed, society at large, observes many important problems in which chemistry is involved and for which chemists should play a dominant role in providing solutions, but which IUPAC does not address.

Of course, IUPAC is an organization with only very limited financial resources. The amount of money available for scientific activities is equivalent to the salary of only a few full-time postdoctoral research assistants in the United States. Nevertheless, IUPAC is still able to play a major role on the international scientific scene, because it is the only global, non-governmental, non-political organization representing chemistry. This unique status gives us a great responsibility, and it is probably the main reason why so many chemists are willing to devote so much time to IUPAC.

In the major part of the 75 years of our existence, great efforts had to be made to maintain communication between chemists. World War II and the subsequent Cold War paralysed many globally co-ordinated efforts. Now that these political barriers have largely disappeared, it is the opinion of the Executive Committee that the Union carefully and critically reconsider its efforts and direction. It is inevitable that the psychological threshold of a new century has also to be mentioned. Where is IUPAC to go, and what is it to do, in the 21st Century?

An important question to be answered is whether the present structure of Divisions and Commissions, which has existed for so long, is still adequate to cope with the complicated scientific problems which society now faces.

The most drastic step proposed in a recent 'brainstorming' session of the Executive Committee was a 'sunset-scenario' – disbanding all Commissions and reinventing the Union.

Another, more popular, approach was to continue our efforts to restructure the Union from its present form. The Applied Chemistry Division (VI) and the Clinical Chemistry Division (VII)/Medicinal Chemistry Section have recently (General Assembly, Guildford) received approval for a change of status to Divisions on *Chemistry and the Environment* and *Chemistry and Human Health*, respectively.

At the same time, we asked the other Divisions to actively enter the discussion on the future direction of the Union.

It would be unjust not to mention that some Divisions and some other scientific bodies within the Union have already made efforts in this direction, by defining new horizons which contribute to the solution of important problems identified by society:

- the CHEMRAWN Conferences have a very high impact rating outside the Union;
- our recent and developing co-operation with UNESCO in projects to help developing countries is very promising, at least three Divisions contribute in this area;
- our efforts towards the solution of environmental problems are appreciated and should be strengthened;
- a few projects now initiated through the Pool of Titular Members address major problems, such as oil spill clean-up and alternative scenarios for future energy production.

Each Division/Section President has been asked to enter this line of thought and contribute to the discussion on where the Union should go and what this could mean for the Divisional structure.

For example, some questions to be addressed could include:

- is the present Commission structure still adequate?;
- should we tackle fewer projects, but with greater intensity and in less time?;
- should we increase the Pool of Titular Members or ask the Divisions to rejuvenate so that this would be unnecessary?.

This was the essential part of the message sent to the Divisions in May.

It was satisfying that at Guildford, notwithstanding the short time available, the Divisions have responded rapidly to this message.

Two new Divisions were created by Council at Guildford, replacing Former Divisions VI, VII and the Medicinal Chemistry Section. Division VI, will from the beginning of 1996, deal with *Chemistry and the Environment*, and Division VII and the Section deal with *Chemistry and Human Health*. Moreover, some Divisions have created a Divisional Pool of Titular Member

positions in order to be able to rapidly initiate projects of an urgent nature.

At this moment, it is not as yet clear whether the projects initiated at Guildford meet the necessary requirements. It is, however, clear that the Divisions are changing. We may look forward to a substantial jump forward in the efforts of the Union to achieve an up-to-date interpretation of its mission as stated in general terms in the statutes.

A lot will depend on the leadership within the Union by Officers, Bureau and Division and Commission Officers. It must be realised however, that leadership within IUPAC is totally different from that in Industry or in a University. In an organisation of volunteers, such as IUPAC, direct orders will not be effective. What is more important is to convince each other on the most appropriate way forward – rather than thinking in hierarchical terms.

The willingness within the Union to renew its scientific activities will not automatically lead to greater visibility of the Union. Considerable thought will have to be given to publicity of the Union. Too little has been done to bring the large amount of outstanding work carried out by the Commissions to the knowledge of the wider chemical community. A thorough investigation of our policy with respect to publicity and publications has to be undertaken in the near future; included in this review should be the rapidly evolving electronic means or world-wide communication.

Another important issue at the General Assembly was the future of the Affiliate Membership Program (AMP). Because of the ever decreasing numbers of affiliates, the Review Panel as well as the Committee on Affiliate Membership came to the conclusion that the continuation of the program could not be justified. A proposal to that effect was not, however, accepted by Council. The Council decided that a small group from the Bureau should investigate the possibility of continuation of the program, possibly in a different form and under a different name. Special attention should be given by this small group to the financial aspects of the program, by looking at means to eliminate the current year-on deficit. Such an investigation will automatically involve future policy with respect to *Chemistry International*. This small group will report to Council in 1997.

At the Bureau meeting directly after the Council, the membership of this small group was established as follows:

- Prof. J.W. Lorimer, Chairman;
- Dr D.F. Eaton;
- Prof. A. Chakravorty;
- Dr J.H. Williams, Secretary.

Council noted with satisfaction that the finances of the Union are in good shape. A moderate increase of the national subscription level, in line with inflation, was accepted.

By the end of this year, many of our colleagues will have completed their term office and will retire from the Union. As many new members will of course join the Union and others will assume new positions.

Prof. K.I. Zamaraev will have completed his term as President and will continue for another two years as Past-President. Prof. A. E. Fischli will assume the office of President of the Union for two years. Prof. J. Jortner, member of the Bureau and the Executive Committee, was elected Vice-President, which means that he will become President from 1 January 1998. Prof. J. M. Ward who had completed his first term of four years as Treasurer was elected for another term office. The post of Secretary General was vacant, and as I did not wish to seek re-election a new Secretary General had to be elected. Dr E. D. Becker, former Chairman of the Committee on Publications, was duly elected Secretary General.

Four vacancies existed for the new Bureau as elected members. Prof. A. Chakravarty (India) was re-elected for another term, and three new Bureau members were elected by Council for four years:

- Prof. P. S. Steyn (Republic of South Africa);
- Prof. G. M. Schneider (Germany);
- Prof. H. Ohtaki (Japan).

After the Council meeting, the Bureau elected, as a new member of the Executive Committee, Prof. P. S. Steyn.

At the end of the year we say farewell, with gratitude for their work for the Union, to: the Past-President, Prof. A. J. Bard; elected Bureau Members Prof. M. T. Beck and Prof. G. Modena; and the Division Presidents Prof. K. Kuchitsu, Prof. K. L. Komarek, Prof. M. Oki, Prof. A. Hulanicki, Prof. H. P. Lehmann and Prof. J. G. Topliss. We welcome as new Division Presidents and Bureau Members:

- Prof. G. Somsen (Physical Chemistry Division);
- Prof. G. J. Leigh (Inorganic Chemistry Division);
- Prof. G. Scorrano (Organic Chemistry Division);
- Prof. M. Gasserbauer (Analytical Chemistry Division);
- Prof. J. Miyamoto (Chemistry and the Environment).

The President of the new Division VII has yet to be appointed, and Prof. J. E. Economy, Macromolecular Division, will act as Chairman of the meeting of Division Presidents.

This concludes my last Secretary General's column. In a couple of months, I will transfer my duties to my successor Ted Becker to whom I wish a very successful term office.

It has been a great privilege to co-operate for so many years with colleagues from all around the world, all of them very much dedicated to our Union. The same applies to the members of the Secretariat, with whom the Secretary General has a special relationship.

Many thanks to you all.

Publications

Fysikaliska grundstorheter	Beteckning för storheten	SI-enhetens namn	SI-enhetens beteckning
längd	*l*	meter	m
massa	*m*	kilogram	kg
tid	*t*	sekund	s
elektrisk ström	*I*	ampere	A
termodynamisk temperatur	*T*	kelvin	K
ämnesmängd substansmängd	*n*	mole	mol
ljusstyrka	I_v	candela	cd

Quantities in Swedish

The Swedish Chemical Society (*Svenska Kemistsamfundet*) has recently produced a Swedish translation of the well know *Abbreviated list of Quantities, Units and Symbols in Physical Chemistry*. The translation has been undertaken by Bertil Holmström.

Copies are available from the Swedish National Adhering Organization: Svenska Nationalkommittén för Kemi, Wallingatan 26B, S-111 24 Stockholm, Sweden.

Liquid Crystals

The Physics of Liquid Crystals by Pierre G. de Gennes, Nobel laureate in physics, was one of the most influential texts on solid state physics of the last 20 years. The author clearly demonstrated the physics fundamental to the dynamics, and the various phase transitions, seen in liquid crystals, and elegantly related such processes to phenomena as disparate as superconductivity. OUP has now brought out a second edition of de Gennes' book, coauthored with J. Prost, the new edition is almost twice the length of the first edition and covers advances made in the field over the last 20 years.

The Physics of Liquid Crystals, *2nd edn, P. G. de Gennes and J. Prost, Oxford University Press, 1993. 597 pp. USD90, ISBN 0-19-852024-7.*

Toxicology in Spanish

The Glossary for chemists of terms used in toxicology (*Pure & Appl. Chem.* **65**(9) 2003–2133 (1993)) has been translated and updated into Spanish: *Glosario de terminos usados en toxicologia*.

The original Glossary was prepared for publication by Dr J. H. Duffus and contained definitions and explanatory notes on over 1200 terms used commonly in the multidisciplinary field of toxicology. The Glossary was prepared primarily for chemists who now found themselves working in toxicology or needed a knowledge of the subject, especially for hazard or risk assessment. Many medical terms were included because of their frequent occurrence in the toxicological literature and because chemists could not be expected to be familiar with them. The Glossary contained two annexes; one containing a list of abbreviations used in toxicology, and one containing a list of abbreviations used by international bodies and by legislation relevant to toxicology and chemical safety.

This Spanish translation of the Glossary has been made by Prof. M. Repetto Jimenez and P. Sanz, of the Institutio Nacional de Toxicología, Departamento Regional, Carretera San Jerónimo, Km 0.4, Apartado Postal 863, 41080 Sevilla, Spain, *in collaboration with C. Jurado, M. López-Artíguez, M. Menéndez and E. de la Peña and is published by the* Asociacion Española de Toxicologia, PO Box 863, 41080 Sevilla, Spain. *Copies of the translation may be obtained from the above, priced USD10.*

Publications from AOAC International

AOAC International is the scientific association dedicated to analytical excellence. It has as its mission, the promotion of methods validation and quality measurements in the analytical sciences.

Since 1884, the Association's primary focus has been the coordination of the development and validation of chemical and microbiological analytical methods by expert scientists working in industry, academic or government laboratories worldwide. These scientists work within three validation programs; the AOAC Official Methods Program, the AOAC Peer-Verified Methods Program and the AOAC Performance Tested Test Kit Program.

AOAC have recently published the 16th edition of their Official Methods of Analysis. This work is the authoritative source of analytical methods used around the world. Volume 1 deals with: Agricultural Chemicals;

Contaminants; Drugs, and Volume 2 with: Food Composition; Additives; Natural Contaminants. In print format, the volumes will be available in January 1995, 1925 pages, 2 volumes, loose-leaf, 237 illustrations, ISBN 0-935584-54-4, USD359 in USA, Canada and Mexico, and USD399 outside North America.

The Official Methods is also available on CD-ROM (after September 1995). USD575 (1 user) in North America and USD595 outside North America.

For further details, please contact: AOAC International, 1970 Chain bridge Road, Department of 0742, Mclean, VA 22109-0742, USA, Fax: +1703 5225468.

AOAC International has recently announced the activation of its World Wide Web Home Page which may be accessed using the Internet address: http://www.aoac.org/.

Latest Edition of the Rubber Handbook

This year marks the 75th Edition of the *CRC Handbook of Chemistry and Physics*, the fifth edition produced during the tenure of David R. Lide as Editor-in-Chief.

The Rubber Handbook has a venerable history. The first edition appeared in 1913, six years before the creation of IUPAC. This first edition contained 116 pages, including advertisements for the laboratory supplies sold by the publisher, the Chemical Rubber Company. The motivation for creating the book was given in its Preface:

In compliance with the requests of hundreds of our friends for a small but comprehensive reference on chemical and physical topics, we have designed and compiled this pocket Manual of Chemistry and Physics. We feel amply rewarded for our effort and expense if this volume proves to be of use and convenience to the profession whose support has been a conscious factor in the growth of our establishment.

It is of interest to note that when this first edition appeared, there were only 81 chemical elements known, the electron had been discovered, however, the nature of the nucleus was as yet a mystery – the neutron was not discovered until 1932 and it was only after this discovery that a full understanding of isotopes could be derived. Madame Curie had just won her second Nobel Prize, however, Max Planck, Niels Bohr and Albert Einstein had yet to be recognised with this honour. Evidently, the evolution of the *CRC Handbook of Chemistry and Physics* has paralleled the growth of modern science and the technological revolution which has followed.

Since the first edition of 1913, the CRC Handbook has been revised annually except for a few years during wartime. It has grown steadily in both size and diversity of information. For example, the 13th edition of 1928 contained 1214 pages in addition to a few advertisements for rubber aprons and stoppers. Nine pages were devoted to wavelengths of atomic spectra, compared to 122 much more closely printed pages in the current edition. The charge on the electron was given, in 1928, to four figures, it is now given to nine figures. The 29th edition of 1945 had reached 2640 pages, with no advertising, but was still in a smaller page format. It included data on amino acids and artificial radioisotopes, and the charge on the electron was given to six figures. Post World War II editions expanded in step with the growth of the scientific establishment, soon leading to the current large page format.

In this thoroughly revised 75th edition, about 80% of the material is different from that published in the 70th edition five years ago. Features of this latest edition include:

- A new, completely revised table of *Physical Constants of Organic Compounds*, covering 12000 compounds.
- Nineteen new or thoroughly revised tables including the following sections:;
- *Thermochemistry*, *Kinetics*, *and Electrochemistry*, including tables of kinetic rate constants for atmospheric chemistry.
- *Fluid Properties*, for example, a new table of vapour pressures of liquids in the ambient temperature range, which lists over 1200 substances;
- *Properties of Solids*, including tables of elasto-optic, electro-optic, and magneto-optic constants as well as elastic constants for single crystals;
- *Geophysics*, *Astronomy*, *and Acoustics*, including updated data on the solar system and geophysical characterisation of the earth.

The users of the Handbook have become as diverse as its contents. It is a standard information source for students beginning at the high school stage, and for professionals. A recent survey showed about 50% of the users are chemists or chemical engineers, with the remainder evenly distributed over physics, biology, materials science, environmental sciences, and the other branches of engineering. The Handbook is widely referenced in the research literature, annual citations typically run close to 2000 distributed over journals in every field of science, and include editions 40 years old.

CRC handbook of Chemistry and Physics, 75th Edition, eds David R. Lide. CRC Press, ISBN 0-8493-0475-X, USD 100.

IUPAC colleague deceased

Prof. J. H. O'Donnell (30 April 1995) – VicePresident of Macromolecular Division (1994–95)/Member of Division Committee (1991–93), Chairman of Australian National Committee for Chemistry

Conferences

14th International Conference on Chemical Education (ICCE) – Chemistry: Expanding the Boundaries
14–19 July 1996
Brisbane, Australia

IUPAC
SPONSORED

This biennial conference, held for only the second time in the southern hemisphere, brings together chemistry teachers, chemists and science educators from school, industry and university settings to share ideas about innovation in the teaching of chemistry. The theme, Chemistry: Expanding the Boundaries, acknowledges the centrality of chemistry through its expanding relationship with many facets of science and everyday life. Conference participants will be challenged to develop this theme with the view of enhancing the relationship between chemistry and other related fields of endeavor. Implications for chemical education beyond 2000 which give a 'science for all' perspective will be encouraged.

The conference will feature plenary lectures, symposia, workshops, poster sessions and exhibitions. The conference language will be English.

The preliminary scientific program includes:

- Implications of research into teaching for chemical education beyond 2000;
- Chemistry: its central purpose in the development of multi-disciplinary approaches to scientific problems;
- Understanding chemistry in the public domain;
- The influence of technology on the nature of chemistry and chemistry education;
- Environmental chemistry: its role in schools and undergraduate *curricula*;
- Chemistry and biotechnology: where to?;
- Designing new molecules and useful materials;
- Evaluating student learning: the influence of national standards;
- Extending the context for learning through industry link programs.

The conference will be located at the St. Lucia Campus of the University of Queensland, located 7 km from the center of Brisbane, the capital of the State of Queens land. The campus is located 18kms from Brisbane airport.

It is anticipated that the registration fee will be AUD500 per person including the conference dinner, lunches, morning and afternoon teas, and the social events. Accommodation costs will be approximately AUD50 per day (bed and breakfast) for university college rooms and from AUD100 per day for hotels.

For further information, please contact: The ICCE Conference Secretariat (Sally Brown), Continuing Professional Education, The University of Queensland QLD 4072, Australia, Tel.: +61 7365 6360, Fax: +61 7365 7099, E-mail: sally@ceu.uq.oz.au

Seventh International Symposium on Solubility Phenomena
22–25 July 1996
Montanuniversität Leoben, Austria

IUPAC
SPONSORED

This symposium will be concerned with many aspects of solubility. There will be plenary lectures by well known specialists and a large number of submitted papers for both oral delivery and poster presentation. The main sections of the meeting will deal with:

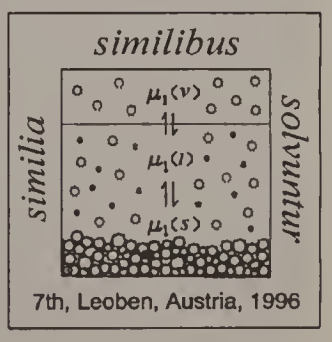
- Electrolyte equilibria and solution thermodynamics;
- Polymers and nonelectrolytes;
- New solubility data and computational aspects;
- Geochemical, industrial and environmental applications;
- Solubility phenomena and metallurgy.

The scientific meeting of the 7th ISSP will be held at Montanuniversität Leoben, Austria. The scientific language of the meeting will be English.

Leoben is the second city of Styria, one of the nine provinces of Austria. The town has a friendly and hospitable atmosphere with many good hotels and restaurants and is situated in a beautiful green landscape surrounded by impressive scenery.

To encourage early registration, the advanced registration fee for scientific participants will be ATS3000 for registrations received before 15 March 1996, thereafter the registration fee will be ATS3500. Student and accompanying person registration is ATS800 before 15 March 1996 and ATS1000 thereafter.

For further information, contact: Dr Erich Königsberger, Symposium Secretary, Abteilung für Physikalische Chemie, Montanuniversität Leoben, A-7800 Leoben, Austria, Fax: +43 3842402 308, E-mail: koenigsb@unileoben.ac.at



14th IUPAC Conference on Chemical Thermodynamics (ICCT-96)
25–30 August 1996
Osaka, Japan

IUPAC
SPONSORED

The conference site will be the Senri Life Science Center, Toyonaka City, which is about 15 kms north of Osaka.

The scientific program will include several plenary lectures and about thirty invited shorter lectures, oral communications and poster presentations. The official language of the conference will be English. It is hoped that there will be a substantial exhibition of scientific instruments, books and databases.

Symposia sessions will discuss:

- Electrolyte and nonelectrolyte solutions;
- Phase equilibria – Equations of state – Fluids;
- Interfaces – Micellar and colloidal systems;
- Inorganic, ceramic and metallic materials;
- Nuclear materials: The 9th International Symposium on Thermodynamics of Nuclear materials;
- Organic and polymeric materials;
- Biological – Medical – Pharmaceutical materials;
- New methods – Data processing – Other topics.

There will be also be a number of workshops, the subject matters to be discussed include:

- Glassy state and relaxation processes;
- Interaction with water;
- Electrochemistry and solid state ionics;
- Pollution and environment.

To encourage early registration, the advanced registration fee for active participants will be JPY30 000 for registrations received before 1 July 1996, thereafter the registration fee will be JPY40 000. Student and accompanying person registration is JPY10 000 before 1 July 1996 and JPY15 000 thereafter.

For further information, please contact: Prof. Michio Sorai, Executive Secretary of ICCT-96, Microcalorimetry Research Center, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan, Tel.: +81 6850 5523, Fax: +81 6850 5526, -5288, E-mail: icct96@chem.sci.osaka-u.ac.jp

CHEMRAWN IX
World Conference on Sustainable Production, Use, Disposal and Recycling of Materials and the Role of Advanced Materials in Sustainable Development
1–6 September 1996
Seoul, Korea

IUPAC
SPONSORED

CHEMRAWN (Chemical Research Applied to World Needs) is one of the more important activities of IUPAC. It is a series of world conferences designed to be high-profile and attract as much publicity as possible in demonstrating the use of chemistry and the chemical industry in solving the more important problems facing humanity.

CHEMRAWN IX will focus on the sustainable production, use, disposal and recycling of material in four important fields. The conference will be composed of plenary and invited lectures, together with poster presentations.

1 *Energy session*

- Energy generation, conversion and storage;
- Fossil energy;
- Nuclear energy;
- Solar energy;
- Fuel energy;
- New energy systems;
- Energy saving processes;
- Membrane separation.

2 *Communication session*

- Memory, storage and display of information;
- Future ICs and computers;
- Optoelectronic materials and systems;
- Multimedia and advanced communications.

3 *Transportation session*

- Future automobiles and technology;
- Electric cars;
- Aerospace and material needs;
- Light weight metal alloys;
- Composite materials.

4 *Construction session*

- Advanced construction materials;
- Wood and wood substitutes;
- Process combination for steel, chemical and coal-based power industries;
- Recycling of materials.

The objectives of the conference will be as follows: (i) To evaluate the current production technology and environmental impacts of materials in the above four areas, viz, energy, transportation, construction and communication. (ii) To clarify the role of technology in reducing the environmental impact imposed by these activities and in developing ecologically sound materials to aleviate their environmental impact. (iii) To elaborate strategies for the selection, and search for, eclogically friendly processes and process combinations involving different industries. (iv) To formulate criteria for the estimation of environmental acceptibility (sustainability) of the present day technologies for materials production. (v) To search for effective means of international cooperation and international imformation exchange in the fields of materials design, production and use. (vi) To formulate a Future Actions Programme, which will enable several of the aforementioned desirable recommendations to be implemented. On the basis of the above, recommendations will be passed to government agencies, international organizations, research groups and industrial leaders.

For registration before 1 May 1996, the full fee will be USD350 and USD75 for a student or an accompanying person. After 1 May 1996, the full registration fee will be USD400 and USD100 for a student or accompanying person. This fee includes the cost of the proceedings and the welcoming party, but not the conferencve banquet.

For further information, please contact: Organizing Committee and Secretariat, IUPAC CHEMRAWN IX, Tongwon B/D 6th Floor, 128-27 Tangju-dong, Chongno-ku, Seoul 110-071 Korea, Tel.: +82(2) 739-4521, Fax: +82(2) 739 6187, E-mail: 5502833@mcimail.com

20th IUPAC Symposium on the Chemistry of Natural Products 15–20 September 1996 Chicago, USA

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As we approach the new millennium, the role of chemistry in understanding our natural environment has been the attention and focus of much debate among scientists and nonscientists alike. The 20th IUPAC Symposium on the Chemistry of Natural Products will provide a unique forum for the discussion and exchange of the latest ideas in this most important and relevant field of research.

The meeting will consist of invited lectures, poster presentations, and a chemical manufacturers/publishers exhibition. Topics that will be covered include:

- Isolation and structure elucidation;
- Synthesis;
- Biomolecules;
- Biotechnology;
- Bio-organic chemistry;
- Role of natural products in industry.

The organizers can arrange accommodation for all participants at the Sheraton Chicago Hotel. Advanced registration will be USD600 for scientists from private organizations, USD500 for scientists from academic laboratories, USD300 for scientists from developing countries, USD150 for students and USD100 for accompanying persons. All these prices, excepting that for accompanying persons, include the cost of breakfast and lunch. The quoted price for accompanying persons includes only breakfast.

Chicago is one of the great cities of the world, and one of the most beautiful in the United States featuring works by some of the greatest 20th-century architects, including Burnham, Sullivan, Wright, van der Rohe and Jahn. Public sculptures by Picasso, Chagall, Miro, Calder and Oldenburg grace the city center. Chicago has several outstanding museums and art galleries, including the Art Institute of Chicago. Many musical festivals run throughout the summer and early autumn, ranging from the well known Jazz/Blues festival in Grant park to the classical series in Ravinia Park.

For further information, please contact: IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, Illinois 60162, USA

Conference Calendar

1996

Phenothiazines and related psychotropic compounds

26–29 February
8th International Conference on Phenothiazines and Structurally Related Psychotropic Compounds. Jaipur, India.
Dr R. R. Gupta, 10A Vasundhara Colony, Tonk Road, Jaipur-30218, India. Tel.: +91 (141) 512694. Fax: +91 (141) 515367.

Chemical physics for the 21st century

16–19 April
International Conference on Chemical Physics on the Border of the 21st Century. Moscow, Russia.
Prof. V. I. Goldanskii, Semenov Institute of Chemical Physics, Russian Academy of Sciences, Kosygin Street 4, Moscow 117977, Russia.

Molecular order in polymers

21–24 May
2nd International Symposium on Molecular Order and Mobility in Polymer Systems. St. Petersburg, Russia.
Prof. T. M. Birshtein, Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoy pr. 31, St. Petersburg, 199004 Russia.

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* **14**, 203 (1992).

Free-radical polymerization

26–31 May.
2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism. Santa Margherita Ligure, Genoa, Italy.
Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy. Tel.: +39 (79) 229556. Fax: +39 (79) 229559.

Mycotoxins and phycotoxins

27–31 May.
9th International Symposiums on Mycotoxins and Phycotoxins. Rome, Italy.
Dr Marina Miraglia, Instituto Superiore Sanità, Food Department, Viale Regina Elena, 299, I-00161 Rome, Italy. Tel.: +39 (6) 4990, ext. 377. Fax +39 (6) 4451767.

Protein folding

17–20 June
International Symposium on Theoretical and Experimental Aspects of Protein Folding. San Luis City, Argentina.
Dr J. Vila, IMASL-Universidad Nacional de San Luis, Ejército de Los Andes 950, 5700 San Luis, Argentina.

Oxidation of polymers

24–28 June
11th Conference on Polymers Thermal and Photo-induced Oxidation of Polymers and its Inhibition in the upcoming 21st Century. High Tatras, Slovak Rrepublic.
Prof. L. Rychlá, Polymer Institute, Slovak Academy of Sciences, Dubravská cesta 9, 842 36 Bratislava, Slovak Republic.

Surface forces

25–29 June
11th International Conference on Surface Forces. Moscow, Russia.
Dr L. B. Boinovich, Institute of Physical Chemistry, Leninsky Prospect 31, 117915, Moscow, Russia.

Organic synthesis

30 June-4 July.
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Conference Secretariat ICOS – 11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (80) 234471. Fax: +31 (80) 601159.

Catalysis

30 June – 5 July.
11th International Congress on Catalysis. Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520–8286, USA. Tel.: +1 (203) 432 4378. Fax: +1 (203) 432 4387.

Chemical education

14–19 July
14th International Conference on Chemical Education – Chemistry: Expanding The Boundaries. Brisbane, Australia.
Dr W. Beasley, Graduate School of Education, The University of Queensland, Brisbane, Queensland 4072, Australia.

Sweeteners

14–20 July
International Symposium on Sweeteners. Jerusalem, Israel.
International Symposium on Sweeteners, PO Box 50006, Tel.:-Aviv 61500, Israel. Tel.: +972 (3) 5140014. Fax: +972 (3) 5175674 or 5140077.

E-mail: 100274.2665@CompuServe.COM.

(Bio)degradable polymers

15–18 July
37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects. Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic.

Solubility phenomena

22–25 July
7th International Symposium on Solubility Phenomena. Leoben, Austria.
Dr E. Königsberger, Symposium Secretary, Abteilung für Physikalische Chemie, Montanuniversität Leoben, A-8700 Leoben, Austria. Fax +43 (3842) 402308. E-mail: koenigsb@unileoben.ac.at.

Macromolecules

4–9 August.
36th International Symposium on Macromolecules. Seoul, Republic of Korea.
Dr Kwang Ung Kim, Secretariat of IUPACMACRO SEOUL'96, Division of Polymers, Korea Institute of Science & Technology, PO Box 131 Cheongryang, Seoul 130–650, Korea. Tel.: +82 (2) 957 6104. Fax: +82 (2) 957 6105. E-mail: iupac@kistmail.kist.re.kr

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy.

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

Excitonic processes

14–17 August
2nd International Conference on Excitonic Processes in Condensed Matter (EXCON '96). Bad Schandau, Saxonia, Germany.
Prof. M. Schreiber, Faculty of Natural Sciences, Technische Universität Chemnitz-Zwickau, D-09107 Chemnitz, Germany.

Coordination chemistry

18–23 August
31st International Conference on Coordination Chemistry. Vancouver, Canada.
31st ICCC Secretariat, UBC Conference Centre, 5961 Student Union Boulevard, Vancouver, BC, Canada V6T 2C9. Tel.: +1 (604) 822 1050. Fax: +1 (604) 822 1069

Macromolecular condensed state

20–25 August
International Symposium on Macromolecular Condensed State. Beijing, China.
Prof. X. Jin, Institute of Chemistry, Chinese Academy of Sciences, PO Box 2709, Beijing 100080, China. Tel.: +86 (1) 02564829. Fax: +86 (1) 02569564. E-mail: huangsl@rose.cnc.ac.cn.

Physical organic chemistry

25–29 August
13th International Conference on Physical Organic Chemistry. Seoul, Republic of Korea.
Prof. J. Suh, Department of Chemistry, Seoul National University, Seoul 151–742, Republic of Korea. Tel.: +82 (2) 8806642. Fax: +82 (2) 8891568.

Biotechnology

25–30 August
10th International Biotechnology Symposium. Sydney, Australia.
10th IBS '96 Symposium Secretariat, GPO Box 128, Sydney, NSW 2001, Australia. Tel.: +61 (2) 2622277. Fax: +61 (2) 2622323. E-mail: veckels@tourhosts.com.au.

Chemical thermodynamics

25–30 August
14th IUPAC Conference on Chemical Thermodynamics. Osaka, Japan.
Prof. M. Sorai, Executive Secretary of ICCT-96, Microcalorimetry Research Center, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan. Tel.: +81 (6) 8505523. Fax: +81 (6) 8505526 (or 5288). E-mail: icct96@chem.sci.osaka-u.ac.jp.

Environmental biotechnology

1–4 September
International Conference on Environmental Biotechnology. Palmerston North, New Zealand.
Conference Secretary, Environmental Biotechnology Conference, Process & Environmental Technology Department, Massey University, Palmerston North, New Zealand. Tel.: +64 (6) 3505351. Fax: +64 (6) 3505654. E-mail: g.f.withers@massey.ac.nz.

CHEMRAWN IX

1–6 September
Sustainable Production, Use, Disposal and Recycling of Materials. Seoul, Korea.
Organizing Committee & Secretariat, IUPAC CHEMRAWN IX, Tongwon B/D 6th Floor, 128–27 Tangju-dong, Chongno-ku, Seoul 110–071, Korea.

Euroanalysis IX

1–7 September
Euroanaysis IX. Bologna, Italy.
Prof. L. Sabbatini, Dipartimento di Chimica, Università di Bari, Via Orabona 4, 70126 Bari, Italy. Tel.: +39 (80) 5442020/16/14. Fax: +39 (80) 5442026.

Characterization of porous solids

15–18 September
4th International Symposium on Characterization of Porous Solids (COPS-IV). Bath, UK
Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, BS19 2FQ, UK. Tel.:. and Fax: +44 (1275) 853311.

Chemistry of natural products

15–20 September
20th IUPAC Symposium on the Chemistry of Natural Products. Chicago, USA.
IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, Chicago, Illinois 60161, USA.

Multiphoton processes

30 September – 4 October
7th International Conference on Multiphoton Processes. Garmisch Partenkirchen, Germany.
Prof. P. Lambropoulos, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany.

Step growth polymerization

September
International Symposium on Step Growth Polymerization, Related Processes and Materials. Paris, France.
Dr B. Sillion, Laboratoire de Chimie Macromoléculaire, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cédex 05, France.
Tel.: +33 (1) 78022078. Fax: +33 (1) 78022010

1997

Thermodynamics

5–8 January
International Symposium on Chemical and Biological Thermodynamics.
Amritsar, India.
Prof. D. V. S. Jain, Department of Chemistry, Panjab University, Chandigarh 160014, India. Tel.: +91 (172) 541435. Fax: +91 (172 541409. E-mail: dvs-jain@imtech ernet.in

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International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
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Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
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Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
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Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
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